PCSI
Room Ballroom South - Session PCSI-MoA2
Topological Materials & Interfaces I

Moderator: Jun Sung Kim, Pohang University of Science and Technology (POSTECH), Republic of Korea

4:30pm **PCSI-MoA2-31 Crystalline Materials with Anisotropic Conduction Polarities*, Joshua Goldberger,*** The Ohio State University **INVITED**

It is conventionally thought is that a single material will exhibit a single kind of conduction polarity, either n-type or p-type, uniformly along all directions of the crystal. Then, in all modern electronic devices, functionality is achieved by integrating together these p-type or n-type materials together. Here we will describe our recent work in the synthesis, properties, and applications of metals and semiconducting materials that exhibit either n-type or p-type conduction behavior depending on the crystallographic direction, a phenomenon we refer to as “goniopolarity”. We will establish the origin of this exotic behavior and the band structure design principles for identifying new goniopolar materials.[1] This has led to a large expansion in the number of compounds that we have experimentally demonstrated to exhibit this effect, such as $NaSn_2As_2$, NaSnAs, WSi_2 and $PdSe_2$.[2-5] Finally, we will show that the unique charge separation in goniopolar materials can overcome limitations of energy-harvesting technologies including thermoelectrics and photocatalysis.

5:10pm **PCSI-MoA2-39 Weyl Semimetals and the Interface: Surface State Transport Probed via Weak Antilocalization in Ultrathin Taas Films*, Ian Leahy,*** *A. Rice, C. Jiang, G. Paul, K. Alberi, J. Nelson,* National Renewable Energy Laboratory

Topological semimetals hold promise for their use in low-powered electronics and spintronic devices [1-4] but these applications await targeted growth on conventional semiconducting substrates and the exploration of their properties in the ultrathin limit. Weak antilocalization (WAL) has been used extensively in the study of surface states in topological insulators and shows promise for the study of surface states in Weyl semimetals (WSMs). WAL is a quantum interference effect that results in an increase in a system’s conductivity owing to the suppression of back-scattering from self-intersecting carrier paths. This quantum interference requires carriers maintain phase coherence over multiple scattering events. The length over which carriers maintain coherence is defined as the decoherence length. In an applied field, the WAL is destroyed when the magnetic length approaches the decoherence length, offering a natural insight into the localizing disorder length scales. Here we report on insights from WAL into the surface state and interface properties of the recently synthesized, single-crystal-like ultrathin films of Weyl semimetal TaAs(001) grown on GaAs(001) substrates [5-7].

Figure 1 shows atomic force microscopy and magnetoconductance for representative TaAs ultrathin films. AFM on a 10 nm thick TaAs film on GaAs reveals oriented, rod-like growth along – the (1\bar10) direction. At low temperatures, the magnetoconductance exhibits clear signatures of WAL. Intriguingly, we find that the number of apparent WAL conduction channels depends on the orientation of the applied current relative to the film topography as well as the number of GaAs/TaAs interfaces. We hypothesize that this unique anisotropic WAL stems from a topological and trivial state with different decoherence lengths localized at each interface.

References:

[1] J. Hu, S. Xu, Z. Mao, Annual Review of Materials Research 49:1, 207-252 (2019).

[2] I. Leahy, et. al., Proceedings of the National Academy of Sciences, 1808747115 (2018).

[3] H. Chorsi, et. al., Advanced Functional Materials, 32:19, 2110655 (2022).

[4] B. Zhao, et. al., Advanced Materials, 32:38, 200818 (2020).

[5] J. N. Nelson et. al., Matter 6, 2886 (2023).

[6] J. Sadowski et. al., Crystal Growth and Design 22, 6039 (2022).

[7] I. A. Leahy et. al., In Revision at ACS Nano (2023).

+Author for correspondence: Ian.Leahy@nrel.gov

5:15pm **PCSI-MoA2-40 Topological Hall Effect in Dirac Semimetal*, Saurav Islam,*** *E. Steinebronn,* Pennsylvania State University*; B. Neupane,* University of North Texas*; K. Yang,* Pennsylvania State University*; Y. Wang,* University of North Texas*; C. Liu,* Pennsylvania State University*; S. Ghosh,* University of Minnesota*; K. Mkhoyan,* University of Minho, Portugal*; J. Chamorro, T. McQueen,* Johns Hopkins University*; N. Samarth,* Pennsylvania State University

Magnetic skyrmions are chiral spin textures whose non-trivial real space topology is often created by an interfacial anisotropic Dzyaloshinkii-Moriya exchange interaction (DMI) that originates from spin-orbit coupling and broken inversion symmetry [1]. They have been observed in a wide variety of bulk single crystals such as MnSi [2] and thin films such as $Fe_{1-x}Co_xSi$ [3]. More recently, magnetic skyrmions have been probed at ferromagnet/topological insulator interfaces [4] and in magnetic Weyl semimetals [5]. This motivates similar explorations of skyrmion formation in Dirac semimetals (DSMs). We investigate the formation of skyrmions at the interface of a canonical DSM (Cd_3As_2) and a ferromagnetic semiconductor ($In_{1-x}Mn_xAs$) with perpendicular magnetic anisotropy. Our calculations indicate nonzero spin susceptibility in such heterostructures due to Rashba spin-orbit coupling from broken inversion symmetry, implying the DM interaction necessary for skyrmions. To experimentally test this idea, we grew $Cd_3As_2/In_{1-x}Mn_xAs$ bilayers (Fig. 1a) and mapped out the behavior of the Hall effect as a function of temperature, magnetic field, and gate voltage in electrostatically top gated devices. Below T = 6 K, we observe an emergent gate-tunable topological Hall effect (THE) indicated by an excess Hall resistance (Fig. 1b). This signature is most pronounced at the charge neutrality point, suggesting the formation of a Dirac-electron mediated chiral spin texture at the DSM/ferromagnet interface. Our study provides a new platform to study the interplay between the topological states in DSMs and the chiral spin textures associated with the THE. Supported by the NSF Graduate Research Fellowship Program (Grant No. DGE1255832).

[1] A. Fert, N. Reyren, and V. Cros, Nat. Rev. Mater., 2, 1 (2017).

[2] S. Mühlbauer et al., Science 323, 915–919 (2009)

[3] X.-Z. Yu et al., Nature 465, 901–904 (2010)

[4] P. Li et al., Nano Lett., 21, 1, 84–90 (2021)

[5] P. Pushpan et al., Phys. Rev. Lett. 124, 017202 (2020)

+Author for correspondence: ski5160@psu.edu, nxs16@psu.edu

5:20pm **PCSI-MoA2-41 Helical Dislocations in 2D Materials and the Connection to Transport in Topological Insulators*, T. Rakib, M. Choi, E. Ertekin,*** University of Illinois at Urbana-Champaign*; P. Pochet,* Universite Grenoble-Alpes, France*; **Harley Johnson**,* University of Illinois at Urbana-Champaign

Layered two-dimensional materials host a variety of crystalline defects, including dislocations either in-plane or out-of-plane with respect to the 2D layered structure. Recently, twisted multilayer 2D material structures have been of interest due to the presence of flat bands and other emergent properties associated with moiré superlattices.[1] Periodic regions of crystalline commensurability making up these superlattices are now understood to be separated by interlayer dislocations, with Burgers vectors and line directions in the plane of the 2D material, and having either edge or screw character.[2] Using density functional theory and quantum Monte Carlo-fitted total energy tight-binding calculations, we show that out-of-plane relaxation of the structures makes possible unique helical dislocations in bilayer graphene, and that the presence of these helical dislocation lines coincides precisely with the so-called magic-angle condition at which unconventional superconductivity is observed.[3] We then illustrate a different dislocation structure, with line direction oriented out-of-plane, but which also has a helical structure. Such a screw dislocation, which adopts a double-helix dislocation core configuration in bilayer structures, is expected to create conditions for exotic transport properties in certain classes of layered topological insulator materials. We present initial results demonstrating this possibility in BiTe and BiSe compounds. In these examples, we present relaxed dislocation core structures computed using first-principles methods, and show that the observed configurations match both experimental observations and the theoretical conditions that are expected to lead to quantum conduction in these otherwise topologically insulating materials.

[1] Cao, Y. et al., Unconventional superconductivity in magic-angle graphene superlattices, Nature **556**, 43-50 (2018).

[2] Pochet, P., B. C. McGuigan, J. Coraux, and H. T. Johnson, Toward moiré engineering in 2D materials via dislocation theory, Applied Materials Today **9**, 240-250 (2017).

[3] Rakib, T., P. Pochet, E. Ertekin, and H. T. Johnson, Helical dislocation in twisted bilayer graphene, Extreme Mechanics Letters, **63**, 102053 (2023).

+ Author for correspondence: htj@illinois.edu

5:25pm **PCSI-MoA2-42 Layer-dependent Optical Conductivity of MBE-grown $ZrTe_2$***, E. Houser,* ***Frank Peiris****,* Kenyon College*; A. Richardella, M. Stanley, N. Samarth,* Pennsylvania State University

Besides providing an interesting platform to interrogate fundamental physics questions, two-dimensional transition metal dichalcogenides (TMDCs) are well suited to advance the development of optoelectronic technologies. In this work, we investigated the growth and the optical properties of $ZrTe_2$, a candidate topological Dirac semimetal, grown using molecular beam epitaxy. During the growth of 12 unit cells (u.c.) of $ZrTe_2$ on a sapphire substrate, we obtained in-situ spectroscopic ellipsometry after the deposition of each u.c. Additionally, we obtained temperature dependent ellipsometry data on the sample between 20 ℃ and 350 ℃. After the deposition of the $ZrTe_2$ layers, a Te capping layer was deposited in order to protect the TMDC film. Post-growth X-ray reflectivity measurements indicated that the total thickness of $ZrTe_2$ and the thickness of Te to be 5.95 nm and 19 nm, respectively.

A standard inversion technique was used to model the ellipsometry spectra by specifying a three layer model (i.e., sapphire substrate, $ZrTe_2$ layer and the Te capping layer) to fit the final ellipsometry spectra. The thicknesses obtained from X-ray reflectivity allowed us to obtain the precise dielectric function of the final $ZrTe_2$ layer (i.e., 12 u.c.), which was converted to the optical conductivity. Subsequently, we fit the remaining ellipsometry spectra obtained for 11 u.c. through 1 u.c. $ZrTe_2$ layers. Clearly, the optical conductivity shows a noticeable change with the thickness of the $ZrTe_2$ layers, where the real part increases with the thickness of $ZrTe_2$, as shown in Fig. 1. The layer-dependent conductivity was further analyzed by incorporating a Drude oscillator to account for free electrons, and two Kramers-Kronig-consistent oscillators to represent the band-to-band transitions. Interestingly, we find that the Drude contribution reduces as the thickness of $ZrTe_2$ gets smaller, suggesting that its metallic character diminishes as the thickness reduces.

5:30pm **PCSI-MoA2-43 Surface Dependent Doping Efficiency in Te:Cd_3As_2 Thin Films***, **Anthony Rice**, I. Leahy, K. Alberi,* National Renewable Energy Laboratory

Cd_3As_2 is a prototypical Dirac semi-metal, a class of materials with gapless topologically protected electronic states. In this system, these topological electronic states are close to the intrinsic Fermi level and are well isolated from non-trivial bands. Additionally, this system is air stable and compatible with molecular beam epitaxy, including lattice matching to III-Sb and II-Te layers, and similar elements to conventional semiconductors. These materials could play a role in a large number of applications, including transistors, spintronics, photodetectors, and thermoelectrics. To do this, however, significant progress must be made on achieving tunability of these materials. In particular, routes to altering its typical n-type carrier concentration must be developed.

Previous attempts to dope Cd_3As_2(112) with group VI elements, including Te and Se, were successful, allowing for increases of n_{3d} from 5e17 cm^{-3} up to slightly over 3e18 cm^{-3} [1]. Concentration vs mobility relationships appeared similar to doping in convention semiconductors, with mobility decreasing with increased ionized impurities. Attempts to increase doping beyond this level by using increased group VI fluxes resulted in lower measured Hall concentrations and even larger decreases in mobility, a sign that compensating defects are forming. When similar doping is attempted on the (001) surface, however, doping beyond 1e19 cm^{-3} is possible. Furthermore, an order of magnitude smaller Te fluxes are required to achieve similar doping levels. Finally, smaller unintentionally doped carrier concentrations are achievable on this surface. This work highlights the role of surface kinetics in defect incorporation in topological semi-metals.

[1] A.D. Rice et al. Appl. Phys. Lett. 122, 061901 (2023)

+Author for correspondence: Anthony.rice@nrel.gov

5:35pm **PCSI-MoA2-44 Investigating the Structural and Electronic Properties of FeSn on $LaAlO_3$(111) Grown by Molecular Beam Epitaxy***, T. Erickson,* ***Sneha Upadhyay****, A. Shrestha, A. Abbas, H. Hall, D. Ingram, S. Kaya, A. Smith,* Ohio University

The Kagome lattice of 3-d transition metals produces exciting electronic excitations through correlated topological phases due to a mixture of the unique geometry and spin-orbit coupling [1,2]. Research into these materials continues to provide insight into electronic properties of Dirac-bands in transition metal materials. FeSn with its Fe3Sn Kagome layers separated by honeycomb Sn¬2 layers provides ample opportunity to study these phenomena. Recent scanning tunneling microscopy (STM) studies into FeSn confirm the expected antiferromagnetic spin order consistent with bulk measurements, demonstrating a ferromagnetic alignment within Kagome layers and antiferromagnetic coupling between separate layers [3,4]. Currently, these findings are for bulk FeSn samples transported to and cleaved in ultra-high vacuum chambers. Here, we perform direct in-situ UHV-STM analysis of FeSn samples as-grown by molecular beam epitaxy. We grew our FeSn on LaAlO3 substrates at temperatures ranging from 450 to 550 °C and Fe:Sn flux ratios of 0.64:1 to 1.52:1. LaAlO3 and FeSn have a lattice match with a difference of only 1%. We also compare the results samples by means of RHEED, XRD, RBS, and AFM. In all cases, smooth streaky RHEED patterns are observed, and from the streak spacing we calculate the in-plane lattice constants which are then complemented by the lattice constants calculated from the XRD spectra. For the case of the 1.52:1 flux ratio, using RHEED we find an a = 5.240 ± 0.017 Å as compared to the expected value for the FeSn lattice parameter a = 5.297 Å [2], and using XRD we find c = 4.436 ± 0.042 Å as compared to the expected c for FeSn = 4.481 Å [2]. In this presentation, we will discuss the lattice parameters as functions of the incident flux ratios as well as the phases and phase purity of the resultant samples. Additionally, AFM and RBS results are used to describe the smoothness and stoichiometry respectively.

This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-FG02-06ER46317.

References

[1] Kang, M., Ye, L., Fang, S. et al. Nat. Mater. 19, 163–169 (2020).

[2] Yin, JX., Zhang, S.S., Li, H. et al. Nature 562, 91–95 (2018).

[3] Li, H., Zhao, H., Yin, Q. et al. Sci Rep 12, 14525 (2022).

[4] Lee, SH., Kim, Y., Cho, B. et al. Commun Phys 5, 235 (2022).

+ Author for correspondence: te467518@ohio.edu

5:40pm **PCSI-MoA2-45 Ultra-quantum Limit Magnetotransport in the Topological Pentatellurides***, **Johanna Palmstrom**, C. Ribeiro, C. Mizzi, L. Winter, S. Thomas,* Los Alamos National Laboratory*; J. Liu, L. Jauregui,* University of California Irvine*; J. Mutch, Q. Jiang, J. Ayres-Sims, J. Chu,* University of Washington*; E. Peterson, J. Zhu,* Los Alamos National Laboratory

With low carrier concentrations and high mobilities, the pentatelluride material family ($HfTe_5$ and $ZrTe_5$) typically have a quantum limit of a few Tesla, making them an ideal platform to study ultra-quantum limit phenomena and magnetic field-induced effects in a three dimensional (3D) Dirac fermion system. In the quantum limit, the magnetic field is strong enough to confine all the electrons to their lowest Landau levels, resulting in a quantized in-plane dispersion, lower effective dimensionality, and a system that is more unstable to electronic correlations. Previous experiments in the pentatellurides have revealed many exotic high-field phenomena including an interaction driven instability [1] and a field induced Lifshitz transition [2]. These materials sit right at the cusp of a strong-to-weak 3D topological phase transition, resulting in a band structure and electronic properties that are extremely sensitive to external tuning parameters such as magnetic field and strain [3]. Consequently, while these systems are promising for the extrinsic control of topological properties, there are many controversies surrounding their intrinsic behavior as the electronic properties depend on the sample growth and preparation conditions [4].

In this work we report on the ultra-quantum limit electronic properties and magnetic field-temperature phase diagram of flux grown, bulk $HfTe_5$ as

revealed by magnetotransport measurements in pulsed magnetic fields up to 65 T (Fig. 1). These samples show a purely insulating resistance vs temperature behavior in zero field. We find a strong and non-monotonic angle dependence of the magnetoresistance and several high field features in the ultra-quantum limit. The interpretation of these features will be discussed during the presentation.

[1] L. Yanwen et al. Nat. Commun. **7**, 12516 (2016)

[2] S. Galeski et al. Nat. Commun. **13**, 7418 (2022)

[3] J. Mutch et al. Sci. Adv. **5**, eaav9771 (2019)

[4] J. Liu et al. arXiv:2304.09072 (2023)

[+]Author for correspondence: jpalmstrom@lanl.gov [mailto:jpalmstrom@lanl.gov]

Author Index

Bold page numbers indicate presenter