PCSI
Room Ballroom South - Session PCSI-ThM
Quantum Materials

Moderator: Kirstin Alberi, National Renewable Energy Laboratory

8:30am **PCSI-ThM-1 Interface-Induced Superconductivity in Quantum Anomalous Hall Insulators***, **Cui-Zu Chang**,* Penn State University **INVITED**

When two different electronic materials are brought together, the resultant interface often shows unexpected quantum phenomena, including interfacial superconductivity and Fu-Kane topological superconductivity (TSC). In this talk, I will first briefly talk about our recent progress on the quantum anomalous Hall (QAH) effect in magnetic topological insulator (TI) multilayers.Next, I will focus on our recent discovery of interfacial superconductivity in QAH/iron chalcogenide heterostructures. We employed molecular beam epitaxy (MBE) to synthesize heterostructures formed by stackingtogethertwo magnetic materials, a ferromagnetic TI with the QAH state and an antiferromagnetic iron chalcogenide (FeTe). We discovered emergent interface-induced superconductivity in these heterostructures and demonstrated the trifecta occurrence of superconductivity, ferromagnetism, and topological band structure in theQAH layer, the three essential ingredients of chiral TSC. The unusual coexistence of ferromagnetism and superconductivity can be attributed to the high upper critical magnetic field that exceeds the Pauli paramagnetic limit for conventional superconductors at low temperatures.The QAH/FeTe heterostructureswith robust superconductivity and atomically sharp interfaces provide an ideal wafer-scale platform for the exploration of chiral TSC and Majorana physics, constituting an important step toward scalable topological quantum computation.

9:10am **PCSI-ThM-9 Surface Passivation in Black Phosphorous/GaAs Ultra-Thin Heterojunctions***, **Peter-Jonas Ela**, Francesca Cavallo, Emma Renteria,* University of New Mexico*; Sadhvikas Addamane,* Sandia National Laboratories

This work focuses on investigating process-structure-property relationships in bP/GaAs ultrathin heterojunction photodiodes, which are excellent candidates for radio-frequency-hard detection of visible-to infrared waves. In particular, the subject of the study is the effect of bP oxidation on the leakage current of the device.

9:15am **PCSI-ThM-10 Electronic and Optical Properties of Lanthanide-Doped Mos$_2$: Impact of Ionic Size and Orbital Configuration Mismatch***, **Hyosik Kang**, Lukas Muechler,* Penn State University

Single-photon emitters (SPEs) are crucial for quantum technologies such as quantum simulation, secure quantum communication, and precision measurements. Two-dimensional transition-metal dichalcogenides (TMDCs) provide an attractive platform for SPEs due to their atomically thin structure, high extraction efficiency, and compatibility with chip-based photonic devices. However, conventional TMDC SPEs emit mainly in the visible range, which limits their use for telecommunication applications that require infrared wavelengths. Lanthanide doping in TMDCs, such as MoS_2, offers a potential solution by introducing sharp, *f* orbital-derived emissions in the infrared range. Yet, the feasibility and impacts of introducing these dopants remain uncertain due to the large ionic radii of the lanthanides.

In this context, we employ density functional theory calculations to investigate the structural, electronic, and optical impact of lanthanide-doped MoS_2 monolayers (Ln=Ce, Er). By evaluating formation energies with adjacent S vacancies, we assess that sulfur vacancies adjacent to Ln sites play a key role in mitigating lattice strain, enabling thermodynamically stable lanthanide incorporation. Charge-state and band structure analysis reveal that *f* orbital-derived defect states and additional host-related states emerge near the band gap, originating from the mismatch of the orbital configuration between the dopant and the host lattice. Furthermore, optical absorption analysis reveals multiple defect- and *f* orbital-related transitions within the band gap range of the host material. Notably, Er_{Mo} exhibits sharp, weak *f-f* optical transitions (0.9-1.1 eV), suggesting the feasibility of defect engineering for SPE. In contrast, Ce_{Mo} shows only defect-related absorption due to its empty *f* shell.

9:20am **PCSI-ThM-11 Molecular Beam Epitaxial Growth and Scanning Tunneling Microscopy Studies of Weyl Semimetals Mn3Ga and Mn3Sn on Hexagonal Wurtzite GaN Substrates***, Hannah Hall, Sunil Timilsina, Ashok Shrestha, Ali Abbas, Sneha Upadhyay, Tyler Erickson, Cherie D'Mello, David Ingram, **Arthur Smith**,* Ohio University

Weyl semimetal systems including Mn_3Ga and Mn_3Sn are known for their fascinating electronic and magnetic properties and effects including anomalous Hall effect, topological Hall effect, giant piezo spintronic effect, large exchange bias, full electronic switching, and more [1, 2, 3, 4, 5, 6] Both Mn_3Ga and Mn_3Sn are non-collinear antiferromagnetic having the Kagome inverse triangular spin structure. We utilize a combination of molecular beam epitaxial growth and *in-situ* scanning tunneling microscopy to investigate high-quality, mirror-like surfaces of these materials and to study the structural, electronic, and magnetic properties of the surfaces using ultimately spin-polarized STM and tunneling spectroscopy.

In the case of Mn_3Ga, we have successfully performed MBE growth on *c*-plane wurtzite GaN and carried out room-temperature STM investigations of the surface, finding smooth spiral growth mounds and a spattering of pinholes on the surface (see Fig. 1). The surface step edges indicate that the structure is hexagonal given the 120° step angles. Atomic resolution images reveal the hexagonal structure with lattice constant $a = 5.60 +/- 0.10$ Å (reported a = 5.4037 Å [4]).

In the case of Mn_3Sn, we grew extremely high-quality films on *c*-plane wurtzite *GaN* grown on sapphire (0001). Reflection high energy electron diffraction and x-ray diffraction were used to determine the *in-plane* and *out-of-plane* lattice constants, respectively. The final determined values were a = 5.670 Å, c = 4.526 Å which are in excellent agreement with ideal expected values (differences from expected are +0.0833% for a and -0.1104% for c, respectively). Preliminary STM results show an atomically smooth surface.

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[3] H. Guo, Z. Feng, H. Yan, J. Liu, J. Zhang, X. Zhou, et al., Adv. Mater. **32**, 2002300 (2020).

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9:25am **PCSI-ThM-12 Band-Bending in Dirac Semi-Metal/Semiconductor Interfaces***, **Anthony Rice**, Ian Leahy, Kirstin Alberi,* National Renewable Energy Laboratory

Cd_3As_2 provides an excellent platform for studying the properties Dirac semi-metals. Electrically, it has a single band crossing well isolated from trivial bands, with an Fermi level that is intrinsically close to the Dirac point. Additionally, its similarity structurally and chemically with III-V and II-VI compounds allow for straightforward combination with semiconductors, creating pathways for high-quality epitaxial integration to utilize the unique properties of topological semimetals. Beyond their stand-alone properties, due to their vanishing density of states near Dirac points, large shifts in the Fermi level may occur from band-bending, creating possibilities for unique charge control at interfaces with implications for devices and even contact layers.

Here, Cd_3As_2/n-GaAs interfaces are first explored. Using molecular beam epitaxy, Cd_3As_2 layers are grown directly on GaAs. Depending on the doping, these Cd_3As_2 layers have a Fermi level 30-100 meV above the Dirac point. Using capacitance-voltage measurements, band alignments are calculated, suggesting a mid-gap alignment of the Dirac point. Due to the large dielectric constant of Cd_3As_2, most of the built-in voltage drop occurs in the n-GaAs layer, giving rise to a Schottky barrier. Attempts at forming rectifying barriers on p-GaAs have resulted in Ohmic junctions, suggesting band-bending in the Cd_3As_2 layer results in the near-interface region becoming p-type. Results with p-CdTe will also be discussed.

9:30am **PCSI-ThM-13 Angle Dependent Magnetoresistance in Cd_3As_2 Thin Films***, **Ian Leahy**, Anthony Rice,* National Renewable Energy Laboratory*; Herve Ness,* Department of Physics, King's College London, UK*; Jocienne Nelson, Mark van Schilfgaarde, Kirstin Alberi,* National Renewable Energy Laboratory

Measurements of the magnetic field angle dependence of magnetotransport have become very popular in the study of topological semimetals, potentially containing information about Fermi surface anisotropy, magnetocrystalline anisotropy, or mobility anisotropy[1-3]. Here, we report on a detailed analysis of angle dependent magnetotransport in (001) Cd_3As_2 thin films of varying carrier densities. We identify a range of possible behaviors depending on mobility and carrier density. Most strikingly, we find a large, positive magnetoresistance (MR) for both and (black trace in Fig. 1), contingent on the direction of the applied current and sample carrier density. In the configuration, this large MR can evolve from negative longitudinal MR at low magnetic fields. Using an 8 x 8 model in a magnetic field and linear response theory, we calculate the theoretical field angle and field magnitude dependence of the longitudinal and Hall resistivities, finding nontrivial dependence on the Fermi energy, which we compare to our experimental results.

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10:00am **PCSI-ThM-19 Atomic-scale identification of Boson Complexes across Heterogenous Interfaces in 2D Materials*, Kory Burns,*** University of Virginia, USA*; Hayden Barry,* University of Virginia*; Christopher Smyth,* Sandia National Laboratories, USA*; Jordan Hachtel,* Oak Ridge National Laboratory, USA **INVITED**

Two-dimensional (2D) compound semiconductors exhibit a range of levels of disorder dependent on their stoichiometry, which can be engineered based on growth conditions, substrate interactions, or atom-by-atom modifications with charged projectiles. There is an entire framework of studies that builds upon research dedicated towards the associated properties with heterogeneities in films, but fail to make one-to-one correlations with the atomic arrangement of the lattice and the optical/infrared emissions. In this talk, we first use aberration-corrected scanning transmission electron microscopy (STEM) to visualize the atomic sites and interfacial growth along semiconducting films. Then, monochromated electron energy loss spectroscopy (EELS) inside an aberration-corrected STEM is used, which greatly reduces the energy distribution of the electron source to maximize the energy resolution without sacrificing too much spatial resolution. Accordingly, we map the high-frequency vibrational modes and exciton complexes in transition metal dichalcogenides (TMDs) moiré structures (Fig. 1) and transition metal monochalcogenides (TMCs) lateral interfaces (Fig. 2). We strategically incorporate off-axis EELS into our workflow, in which it suppressed delocalized responses from Cherenkov radiation losses, to correlate the impact single atom modifications have on the vibrational and optical spectrum. Ultimately, we address applications ranging from magnetic-tunnel transistors to energy harvesting devices.

10:40am **PCSI-ThM-27 Correlated Electron States in Multilayer Graphene: From Superconductivity to Half-Integer Quantum Hall Effects*, Mark Bockrath,*** Ohio State University **INVITED**

Thin graphite flakes behave as two-dimensional conductors in sufficiently high magnetic fields, with quantum Hall states extended throughout the bulk of the flake for low doping, and confined to the surfaces for large doping. I will discuss our observation of half-integer fractional quantum Hall states at large total filling factors. These single-component states likely stem from Pfaffian wavefunctions derived from those in graphene bilayers, which are predicted to host nonabelian quasiparticles. The facile integration of graphite with top and back surface gates makes this an excellent system to explore device geometries capable of manipulating such quasiparticles. Moreover, the group velocity v_F of the electrons in a flat band superconductor is extremely slow, resulting in quenched kinetic energy. Superconductivity thus appears impossible, as conventional theory implies a vanishing superfluid stiffness, coherence length, and critical current. Using twisted bilayer graphene (tBLG), we explore the profound effect very small v_F in a superconducting Dirac flat band system. We find an extremely slow $v_F\sim$ 1000 m/s for filling fraction between -1/2 and -3/4 of the moiré superlattice. This velocity yields a new limiting mechanism for the superconducting critical current, with analogies to a relativistic superfluid. We estimate the superfluid stiffness, which determines the electrodynamic response of the superconductor, showing that it is not dominated by the kinetic energy, but by the interaction-driven superconducting gap, consistent with recent theories on quantum geometric contributions. Finally, we have shown that incompressible states form at 1/3 fractional filling factors in twisted bilayer graphene at angles larger than the magic one that are strongly dominant over integer fillings. These results are in agreement with a strong-coupling theory based on Coulomb interactions between electrons occupying three-lobed Wannier orbitals, leading to novel symmetry-broken phases with distinct charge, spin, and valley order.

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