2D Materials Technical Group
Room C123 - Session 2D1-ThA

2D-Materials: Topological and Quantum Properties

Moderators: Harriet Åhlgren, University of Vienna, **Miaofang Chi**, Oak Ridge Natinal Laboratory

2:20pm **2D1-ThA-1 2D Transition Metal Chalcogenide Semimetals*, David Cobden,*** University of Washington **INVITED**

Graphite (graphene) is a 2D semimetal that after nearly two decades still continues to surprise. Only one other 2D semimetal, WTe_2, has been studied in detail down to the monolayer limit, where it too exhibits diverse properties including topological edge conduction, superconductivity, ferrolectricity, and probable excitonic order. The indications are therefore that 2D semimetals in general form an extraordinarily rich class of materials that deserves more exploration. We will talk about our ongoing work to understand the properties of monolayer WTe_2 better, to investigate the hybrid semimetal system of graphene/WTe_2, and to isolate and study other semimetallic 2D transition-metal chalcogenides.

3:00pm **2D1-ThA-3 Artificial Graphene Nanoribbons with Tailored Topological States*, Nathan Guisinger,*** *P. Darancet,* Argonne National Laboratory, USA

Low-dimensional materials functioning at the nanoscale are a critical component for a variety of current and future technologies. From the optimization of light harvesting solar technologies to novel electronic and magnetic device architectures, key physical phenomena are occurring at the nanometer and atomic length-scales and predominately at interfaces. In this presentation, I will discuss low-dimensional material research occurring in the Quantum and Energy Materials (QEM) group at the Center for Nanoscale Materials. Specifically, the synthesis of artificial graphene nanoribbons by positioning carbon monoxide molecules on a copper surface to confine its surface state electrons into artificial atoms positioned to emulate the low-energy electronic structure of graphene derivatives. We demonstrate that the dimensionality of artificial graphene can be reduced to one dimension with proper "edge" passivation, with the emergence of an effectively-gapped one-dimensional nanoribbon structure. Remarkably, these one-dimensional structures show evidence of topological effects analogous to graphene nanoribbons. Guided by first-principles calculations, we spatially explore robust, zero-dimensional topological states by altering the topological invariants of quasi-one-dimensional artificial graphene nanostructures. The robustness and flexibility of our platform allows us to toggle the topological invariants between trivial and non-trivial on the same nanostructure. Our atomic synthesis gives access to nanoribbon geometries beyond the current reach of synthetic chemistry, and thus provides an ideal platform for the design and study of novel topological and quantum states of matter.

3:20pm **2D1-ThA-4 Critical Materials: Fine Tuning Electronic and Structural Properties of Rare-Earth Based 2-D Structures at the Atomic Limits*, Kyaw Zin Latt,*** Nanoscience and Technology Division, Argonne National Laboratory*; T. Ajayi,* Nanoscience and Technology Division, Argonne National Laboratory ; Nanoscale and Quantum Phenomena Institute, and Department of Physics & Astronomy, Ohio University*; X. Cheng,* Department of Chemistry and Biochemistry, Ohio University*; N. Dandu,* Materials Science Division, Argonne National Laboratory*; A. Ngo,* Materials Science Division, Argonne National Laboratory; Chemical Engineering Department, University of Illinois*; E. Masson,* Department of Chemistry and Biochemistry, Ohio University*; S. Hla,* Nanoscience and Technology Division, Argonne National Laboratory; Nanoscale and Quantum Phenomena Institute, and Department of Physics & Astronomy, Ohio University

Rare-earth metals have many important applications including quantum information, energy up-conversion, emission, and catalysis. In the rare-earth based molecules, the interaction between the metal atom and local electronic states plays a vital role in determining its properties. This can be exploited by engineering molecular ligands to tailor for desired applications. These molecular ligands not only protect the rare-earth metal atoms from the surrounding environment but also influence electronic and magnetic properties [1,2]. Thus, they can be used to tailor the properties of rare-earth ions. Based on the design of the ligands, it can form different types of self-assembled structures which further opens the opportunity to fine tune the properties. In our research, we have designed a variety of rare-earth (Eu,Tb,La) based molecular systems which are deposited onto noble metal surface such as Au(111) under ultrahigh vacuum(UHV) environment to form self-assembled 2D layers. Using a low temperature scanning tunneling microscope, atomic level characterizations of electronic and structural properties of rare-earth complexes absorbed on metal surfaces are performed. Furthermore, tunneling spectroscopic mapping of a self-assembled cluster reveals the spatial variation of electronic orbitals. The experimental results are supported by density functional theory calculations.

[1]. T.M. Ajayi, V. Singh, K.Z. Latt, S. Sarkar, X. Cheng, S. Premarathna, N.K. Dandu, S. Wang, F. Movahedifar, S. Wieghold, N. Shirato, V. Rose, L.A. Curtiss, A.T. Ngo, E. Masson, & S.-W. Hla. *Atomically precise control of rotational dynamics in charged rare-earth complexes on a metal surface.**Nat. Commun.*** **13**, 6305 (2022).

[2]. T. M. Ajayi, N. Shirato,T. Rojas, S. Wieghold, X. Cheng, K. Z. Latt, D. J. Trainer, N. K. Dandu, Y. Li, S. Premarathna, S. Sarkar, D. Rosenmann, Y. Liu, N. Kyritsakas, S. Wang, E. Masson, V. Rose, X. Li, A. T. Ngo, & S.-W. Hla. *Characterization of just one atom using synchrotron x-rays.**Nature*** (2023) in press.

3:40pm **2D1-ThA-5 Quantum Sensing with Spin Qubits in Hexagonal Boron Nitride*, Tongcang Li,*** Purdue University **INVITED**

The recent discovery of spin qubits in hexagonal boron nitride (hBN), a van der Waals (vdW) layered material, has opened up exciting possibilities for quantum sensing. Owing to its layered structure, hBN can be easily exfoliated and integrated with various materials and nanostructures for in-situ quantum sensing. In this talk, I will provide a brief overview of recent advancements in quantum sensing and imaging using spin defects in hBN [Advances in Physics: X, 8, 2206049 (2023)] and discuss our contributions to this emerging field. We have demonstrated high-contrast plasmon-enhanced spin defects in hBN for quantum sensing [Nano Letters 21, 7708 (2021)] and investigated their excited-state spin resonance [Nature Communications, 13, 3233 (2022)]. Additionally, we achieved optical polarization and coherent control of nuclear spins in hBN at room temperature [Nature Materials 21, 1024 (2022)], paving the way for manipulating nuclear spins in vdW materials for quantum information science and technology applications. Finally, we will discuss our work on sensing paramagnetic ions in water using hBN spin defects [arXiv:2303.02326], which demonstrates the potential of ultrathin hBN quantum sensors for chemical and biological applications.

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