PCSI
Room Ballroom South - Session PCSI-ThM2
2D Materials and Graphene II

Moderator: Scott Crooker, Los Alamos National Laboratory

11:00am **PCSI-ThM2-31 UPGRADED: Reduced Metal Contact Resistances for Moire MoS_2 Interfaces**, ***John Robertson,*** Cambridge University, UK

We show how rotational Moire interfaces for electrical contacts between metals and monolayer MoS_2 can create weakly bonded physisorptive interface sites with weaker Fermi-level pinning. This creates smaller n-type Schottky barrier heights, giving the lowest contact resistances for In and a noble metal Ag, as seen experimentally, but previously unexplained. Analogous sites are found for p-type interfaces on WSe_2.

Scaling of semiconductor devices requires lower contact resistances by reducing Schottky barrier heights (SBH) for metals on transition metal dichalcogenide (TMD) contacts. Duan [1] achieved unpinned Fermi levels and physisorbed interfaces by using metal films mechanically transferred onto unmanufacturable exfoliated MoS_2. This effectively increases the interfacial bond length and makes physisorbed interfaces [2]. We suggest longer bonds can be formed by making Moire interfaces between contacts and TMDs.

The TMD lattice allows an alternative way to create longer interfacial bonds using Moire interfaces. These apply a rotational twist between MoS_2 layer and the metal contact layer [2]. There are three types of interface, on-top site (T), a hollow site (H), and Moire sites (M), Fig. 1. We calculate the interfacial binding energy of each metal interface, and find the most stable configuration, as a function of metal work function ϕ.The data shows two zones of physi- or chemi-sorptive interfaces. We then calculate SBHs for the various bonding sites for each contact metal and show these as a function of ϕ. The previous scattered pattern of SBHs sorts into two trends; most SBHs have a slope with ϕ of 0.24 for T or H interfaces. But Moire sites have a clear depinning trend for E_F, with the slope increasing to 0.37 (Fig. 2). This gives a small n-SBH to the MoS_2 conduction band, and lower contact resistances for In and Ag, as seen experimentally. Similar results are found for p-contacts on WSe_2.

[1]Y Liu…X Duan et al, Nature 393 696 (2017);[2] Z Zhang, et al, ACS AMI 14 11903 (2022)

11:20am **PCSI-ThM2-35 UPGRADED: A Generalized and Modular Approach to Tunnel-Junction Spectroscopy for Quantum Systems**, *M. Kavand, Z. Phillips, M. Hamilton, E. Perez-Hoyos,* The Ohio State University*; D. Freedman,* Massachusetts Institute of Technology*; M. Flatté,* University of Iowa*; J. Gupta,* ***Ezekiel Johnston-Halperin,*** The Ohio State University

We present a generalized and modular scheme for tunneling spectroscopy of 0D quantum systems based on the exfoliation and stacking of 2D heterostructures. In this scheme, layers of graphene/graphite (gr) and hexagonal boronitride (hBN) are assembled into a gr/hBN/hBN/gr tunnel junction. The differential conductance (dI/dV) of this structure is sensitive to both direct tunneling through the insulating hBN and resonant tunneling through any impurity states within the bandgap. As a proof of principle, we demonstrate the ability to resolve a variety of structural defects in hBN as well as the direct observation of the HOMO and LUMO states of vanadyl pthalocyanine (VOPc) encapsulated at the interior hBN/hBN interface of the heterostructure (Fig. 1). The VOPc tunneling spectra directly correlate with scanning tunneling microscopy (STM) of witness samples and are consistent with density functional theory (DFT) of VOPc. This technique is extensible to a wide variety of 0D systems encapsulated at the hBN/hBN interface, including electrically (or redox) active molecular systems, adatoms, and point defects in 2D materials. This generality and flexibility provides an exciting opportunity for both electronic/structural characterization of these quantum states as well as potential applications in quantum information.

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