Reduced Metal Contact Resistances for Moire MoS_2 Interfaces

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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)

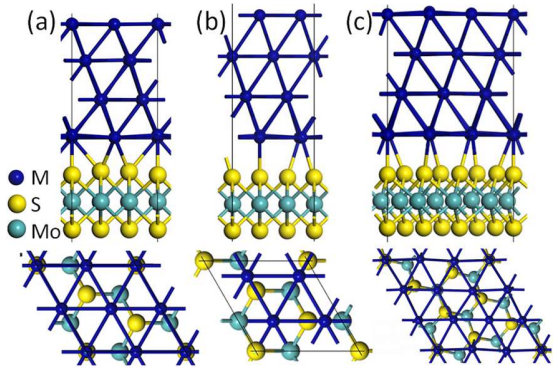

Fig. 1(a) Side and top view of on-top (b) hollow and (c) Moire interfacial sites.

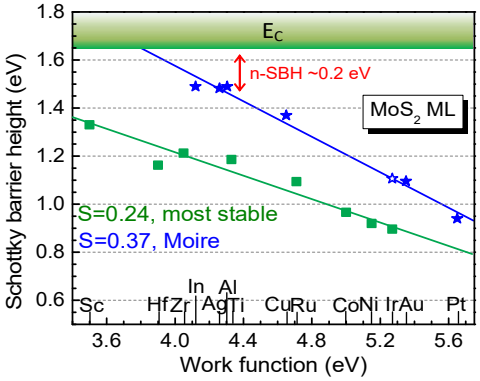

Fig. 2. SBH fit of T,H sites, and of M sites with only physisorption, omitting stars for Co, Ni. Ef depinning factor varies from 0.20 to 0.37.