Supporting On-Line Information for:

Degenerately Doped Transition Metal Dichalcogenides as Ohmic Homojunction Contacts to Transition Metal Dichalcogenide Semiconductors

Zhibin Gao,[†,‡] Zhixian Zhou,[¶] and David Tománek[*,†,§]

†*Physics and Astronomy Department, Michigan State University, East Lansing, Michigan 48824, USA*

‡*Center for Phononics and Thermal Energy Science, School of Physics Science and Engineering, Tongji University, 200092 Shanghai, P. R. China*

¶*Physics and Astronomy Department, Wayne State University, Detroit, Michigan 48201, USA*

§*Mandelstam Institute for Theoretical Physics and School of Physics, University of the Witwatersrand, 2050 Johannesburg, South Africa*

E-mail: tomanek@pa.msu.edu

Supercells representing the MoO_3/MoS_2 bilayer

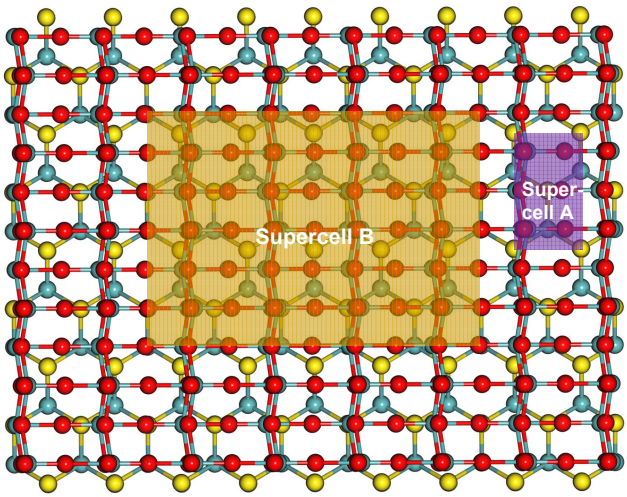

Figure S1: Supercells used to represent the MoO_3/MoS_2 bilayer. The smaller supercell A contains 14 atoms and the larger supercell B contains 156 atoms in total.

Since isolated MoO_3 and MoS_2 monolayers are incommensurate, we approximate the structure of the MoO_3/MoS_2 bilayer by a supercell geometry. We distinguish between the smaller supercell A with 14 atoms, which allows for a simpler interpretation of the results, and the larger supercell B with 156 atoms, which is less strained. The two supercells are shown in Fig. S1.

Effect of the DFT exchange-correlation functional on the electronic structure of MoO_3/MoS_2 and MoO_2/MoS_2 bilayers

By construction, the DFT approach is expected to correctly represent only the total charge density, including charge transfer, and the total energy. Kohn-Sham eigenvalues, which in reality are merely Lagrange multipliers used to minimize the total energy, are commonly used to interpret electronic band structure, even though this interpretation is not well established. Dif-

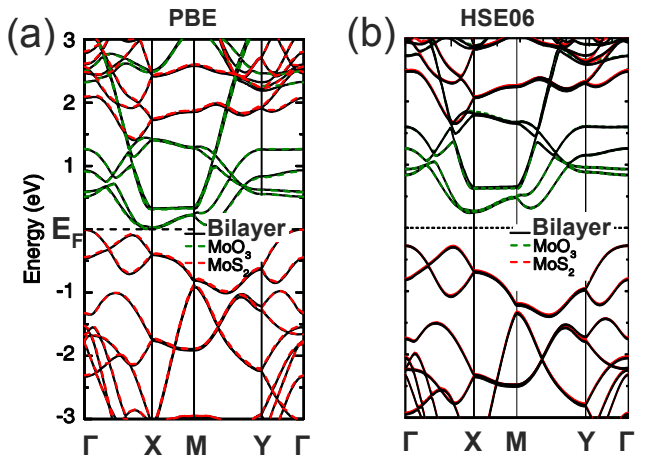

Figure S2: Comparison of the electronic band structure of an MoO_3/MoS_2 bilayer represented by supercell A, obtained using (a) DFT-PBE and (b) DFT-HSE06. Band structure results for the bilayer are compared to those of free-standing monolayers. Panel (a) is equivalent to Fig. 3(c) in the main manuscript.

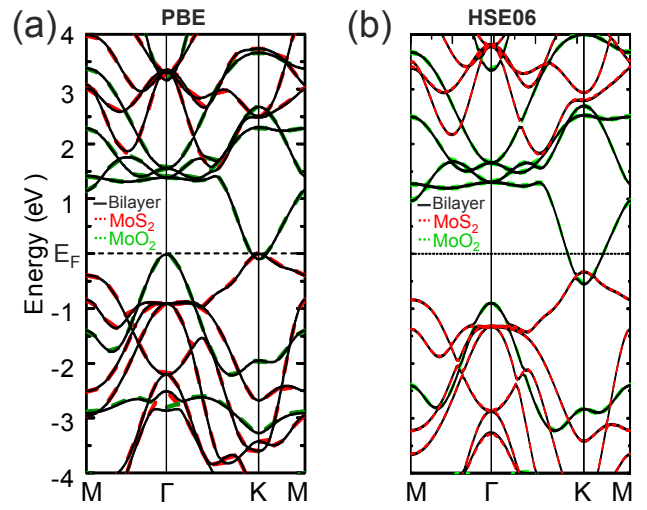

Figure S3: Comparison of the electronic band structure of an MoO_2/MoS_2 bilayer, obtained using (a) DFT-PBE and (b) DFT-HSE06. Band structure results for the bilayer are compared to those of free-standing monolayers. Panel (a) is equivalent to Fig. 8(c) in the main manuscript.

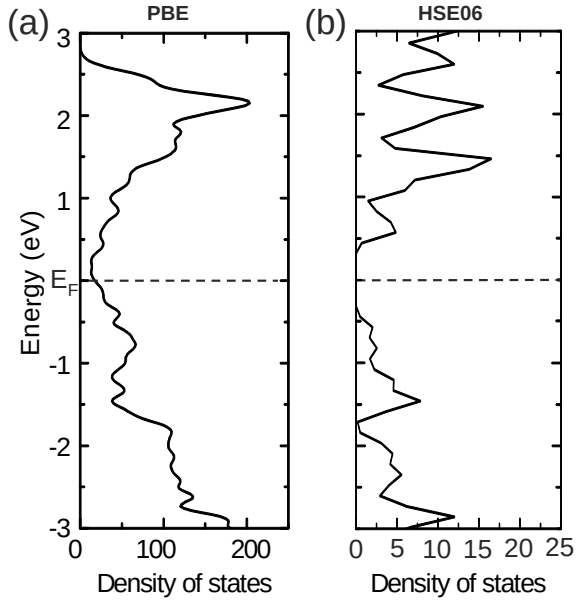

Figure S4: Comparison of the electronic density of states in an MoO_3/MoS_2 bilayer with supercell A based on (a) DFT-PBE and (b) DFT-HSE06. Panel (a) is equivalent to Fig. 5(d) in the main manuscript.

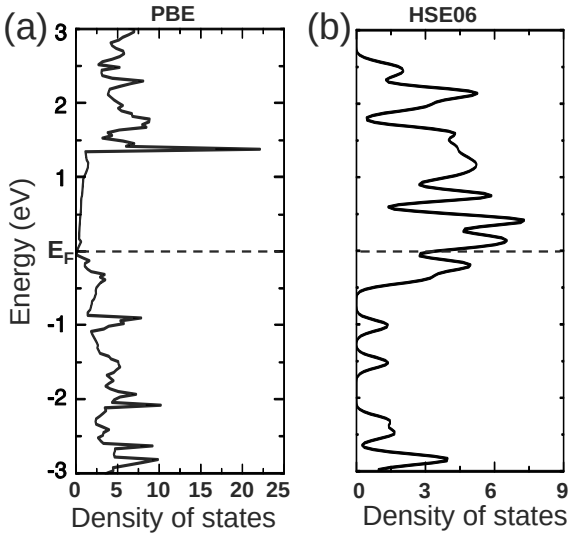

Figure S5: Comparison of the electronic density of states in an MoO_2/MoS_2 bilayer based on (a) DFT-PBE and (b) DFT-HSE06. Panel (a) is equivalent to Fig. 9(d) in the main manuscript.

ferent approaches have been used to describe the contribution of electron exchange and correlation to the Kohn-Sham hamiltonian. Here we compare Kohn-Sham band structures and densities of states based on the widely accepted DFT-PBE nonlocal functional to those based on the hybrid DFT-HSE06 functional. Results for the MoO_3/MoS_2 bilayer are presented in Fig. S2 and Fig. S4, and results for the MoO_2/MoS_2 bilayer are shown in Fig. S3 and Fig. S5. Interpretation of the results is provided in the main manuscript.

We should note that DFT-HSE06 energy eigenvalues presented here depend sensitively on the value of the mixing parameter between DFT-PBE and Hartree-Fock exchange functionals. A much more proper way to determine the electronic band structure would be to solve the self-energy equation, which is computationally very demanding and exceeds the scope of our study.