Supplementary Information

Achieving superlubricating ohmic sliding electrical contact via 2D heterointerface: A computational investigation

Aisheng Song[1], Lei Gao[2], Jie Zhang[1], Xiao Liu[1], Yuan-Zhong Hu[1], Tian-Bao Ma[1*], Quanshui Zheng[1,3], and Jianbin Luo[1*]*

[1]State Key Laboratory of Tribology, Tsinghua University, Beijing 100084, China

[2] Beijing Advanced Innovation Center for Materials Genome Engineering, Institute for Advanced Materials and Technology, University of Science and Technology Beijing, Beijing 100083, China

[3]Department of Engineering Mechanics, Center for Nano and Micro Mechanics, Applied Mechanics Laboratory, Tsinghua University, Beijing 100084, China

Corresponding Author

[*]E-mail: mtb@mail.tinghua.edu.cn
[*]E-mail: gaolei@ustb.edu.cn
[*]E-mail: luojb@mail.tinghua.edu.cn

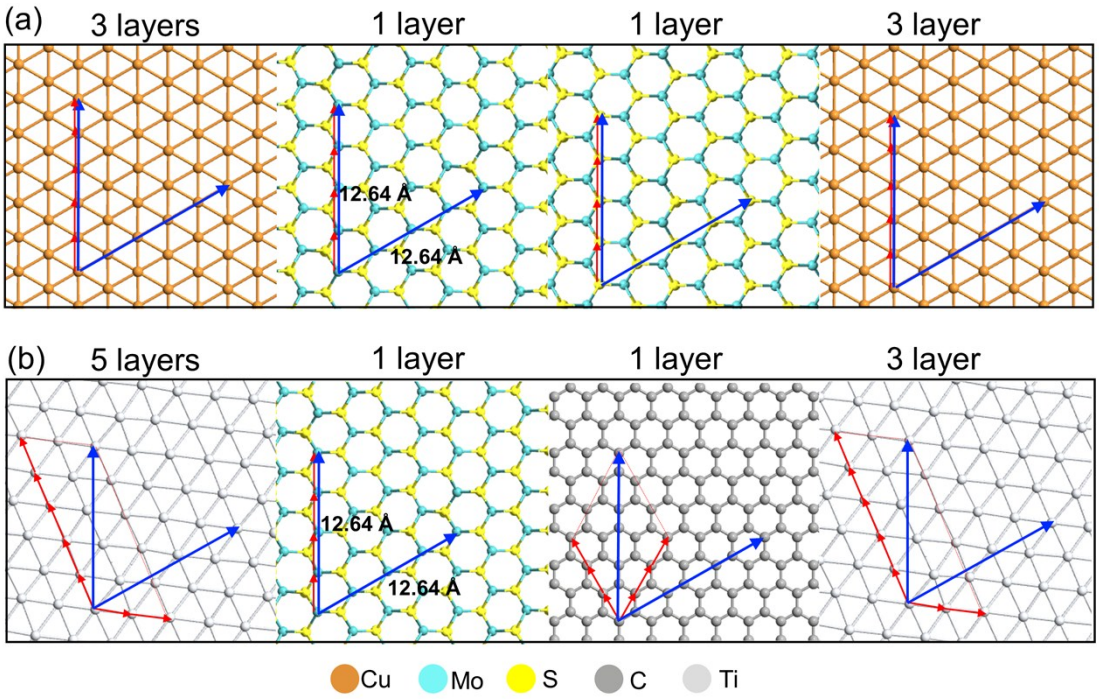

Figure S1. Constructing the Cu-MoS_2-MoS_2-Cu (a) and Ti-$MoS_{1.5}$-Gr-Ti (b) contact systems. The red arrows represent for the lattices of the unit cells while the blue ones represent for the lattices of the supercells. The layer number of metal atoms and 2D materials are marked above the atomic configurations. The Cu-MoS_2-MoS_2-Cu and Ti-$MoS_{1.5}$-Gr-Ti contact systems were constructed by stacking the supercells from left to right.

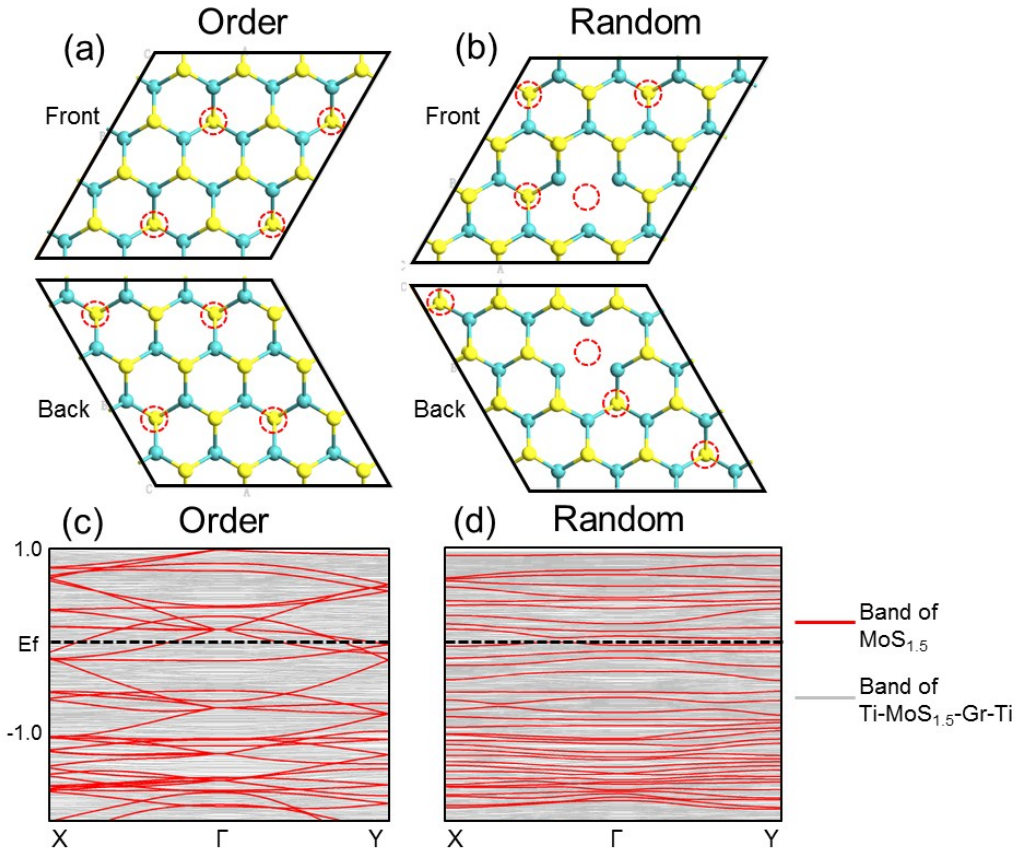

Figure S2. (a)-(d) The atomic configurations and band structures of $MoS_{1.5}$ with orderly (a)(c) and randomly (b)(d) distributed S-vacancies. The S-vacancies are marked by the red dashed circles. The band structures of $MoS_{1.5}$ are aligned to the one of corresponding Ti-$MoS_{1.5}$-Gr-Ti contact systems. The band structures of $MoS_{1.5}$ both showing a zero-bandgap feature, indicating that the Schottky barrier can be eliminated regardless of the S-vacancies distribution.

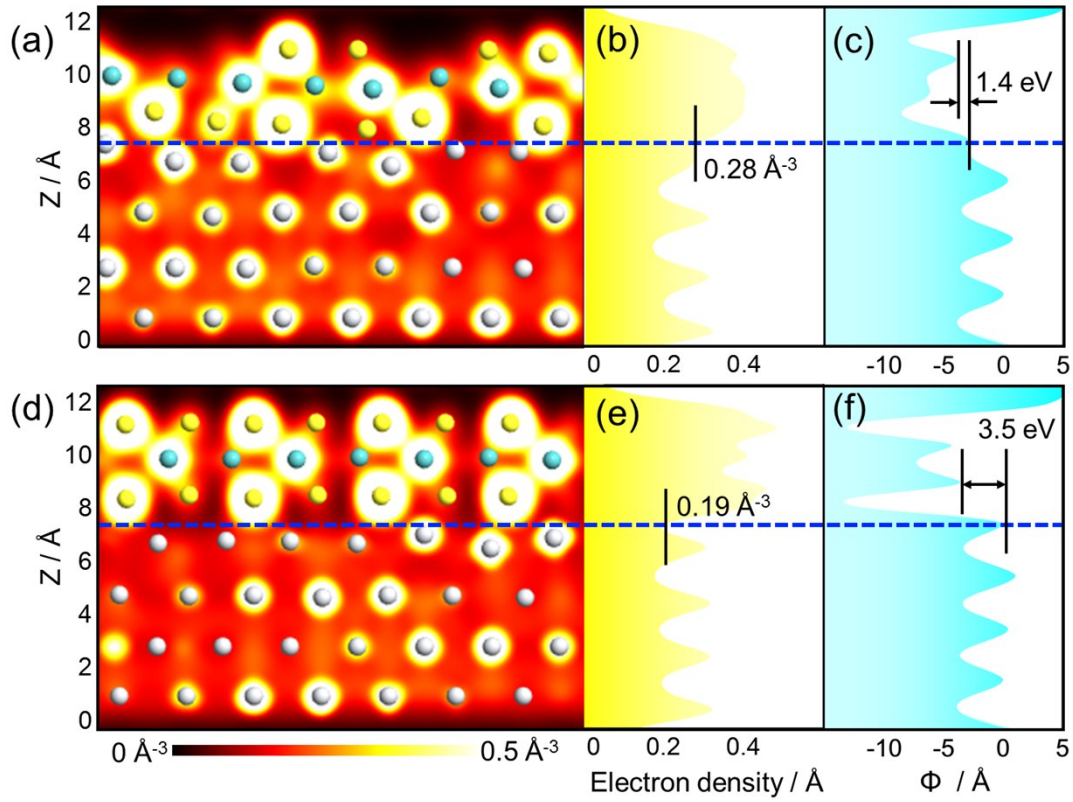

Figure S3. (a)(d) The electron density of $Ti/MoS_{1.5}$ (a) and Ti/MoS_2 contact (d) systems. (b)(c)(e)(f) The electron density distribution (averaged in x-y planes) and electrostatic potential Φ distribution (averaged in x-y planes) of $Ti\text{-}MoS_{1.5}\text{-}Gr\text{-}Ti$ system (b)(c) and $Ti\text{-}MoS_2\text{-}Gr\text{-}Ti$ system (e)(f). The averaged electron density at the $Ti/MoS_{1.5}$ interface is ~50 % higher than that at the Ti/MoS_2 interface, indicating the orbital hybridization is enhanced by the S-vacancy defects, which is favorable to reduce the tunneling barrier[1]. As a result, the tunneling barrier at the $Ti/MoS_{1.5}$ interface is 60% lower than that at the Ti/MoS_2 interface, indicating a higher electron transport transparency.

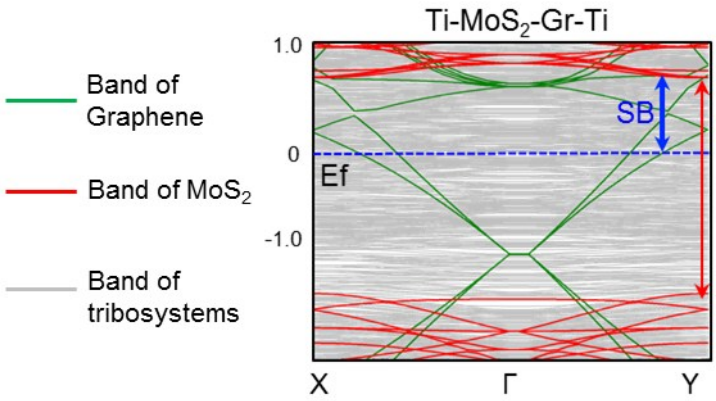

Figure S4. The band structures of Ti-MoS_2-Gr-Ti contact systems. The band structures of MoS_2 are colored by red, graphene by green and aligned to the band structures of the contact systems. The Schottky barrier is ~ 0.6 eV, according to the definition in ref. 2.

References

1. Kang J, Liu W, Sarkar D, Jena D, Banerjee K. Computational Study of Metal Contacts to Monolayer Transition-Metal Dichalcogenide Semiconductors. Physical Review X. 2014;4(3):14

2. Farmanbar M, Brocks G. First-principles study of van der Waals interactions and lattice mismatch at MoS2/metal interfaces. Physical Review B. 2016;93(8): 085304