Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting information

Gate-tunable interfacial properties of in-plane ML MX_2 1T'-2H heterojunctions

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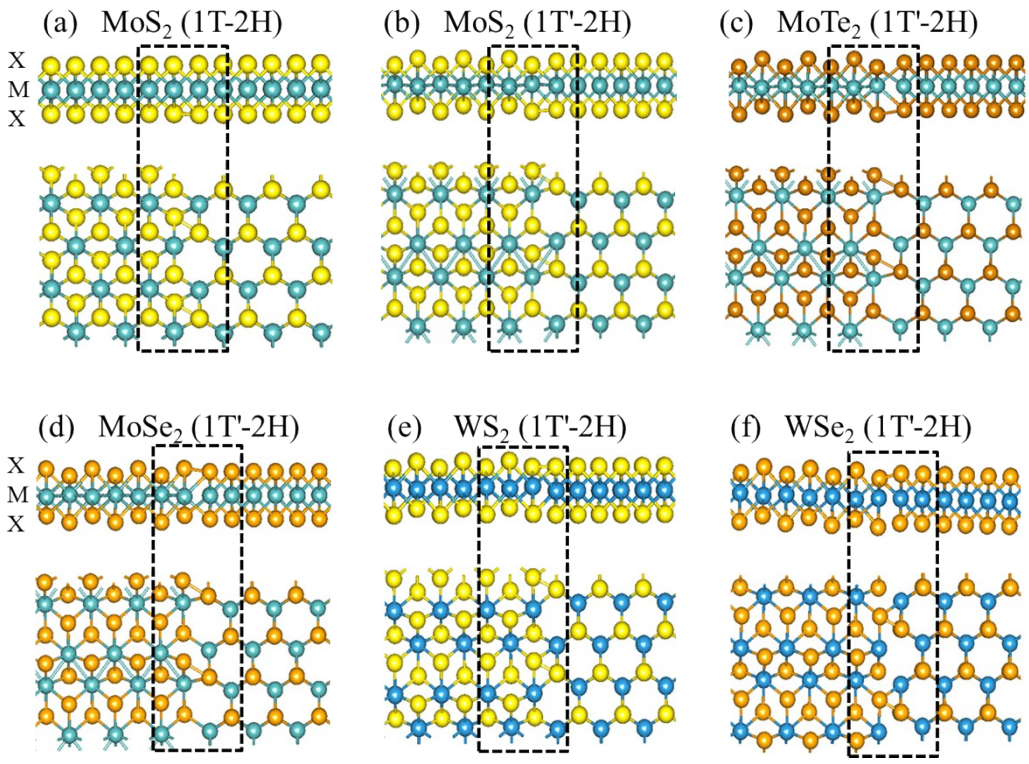

Figure S1. (a) ~ (f): Interfacial structures of the contact configuration for the ML MoS_2 1T-2H in-plane and the ML MX_2 1T'-2H in-plane heterojunctions before optimization. The 1T'/1T and 2H phase within one period at the interface are zoomed in the rectangle black dash line.

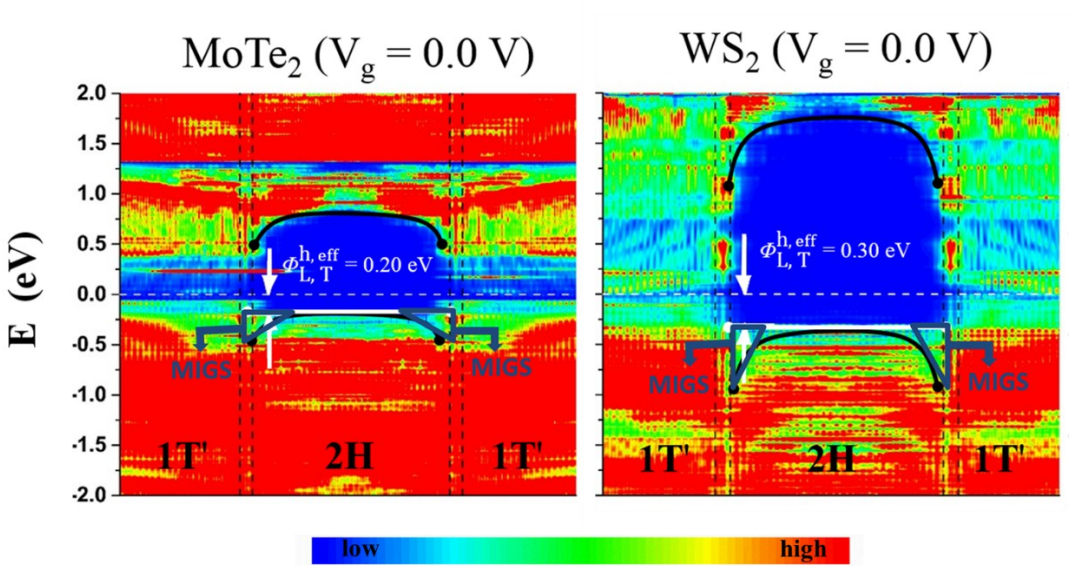

Figure S2: Energy- and space-dependent typical charge density of the MIGS in the ML $MoTe_2$ and WS_2 1T'-2H in-plane heterojunctions. The MIGS at the interface are circled by the dark blue right triangle.

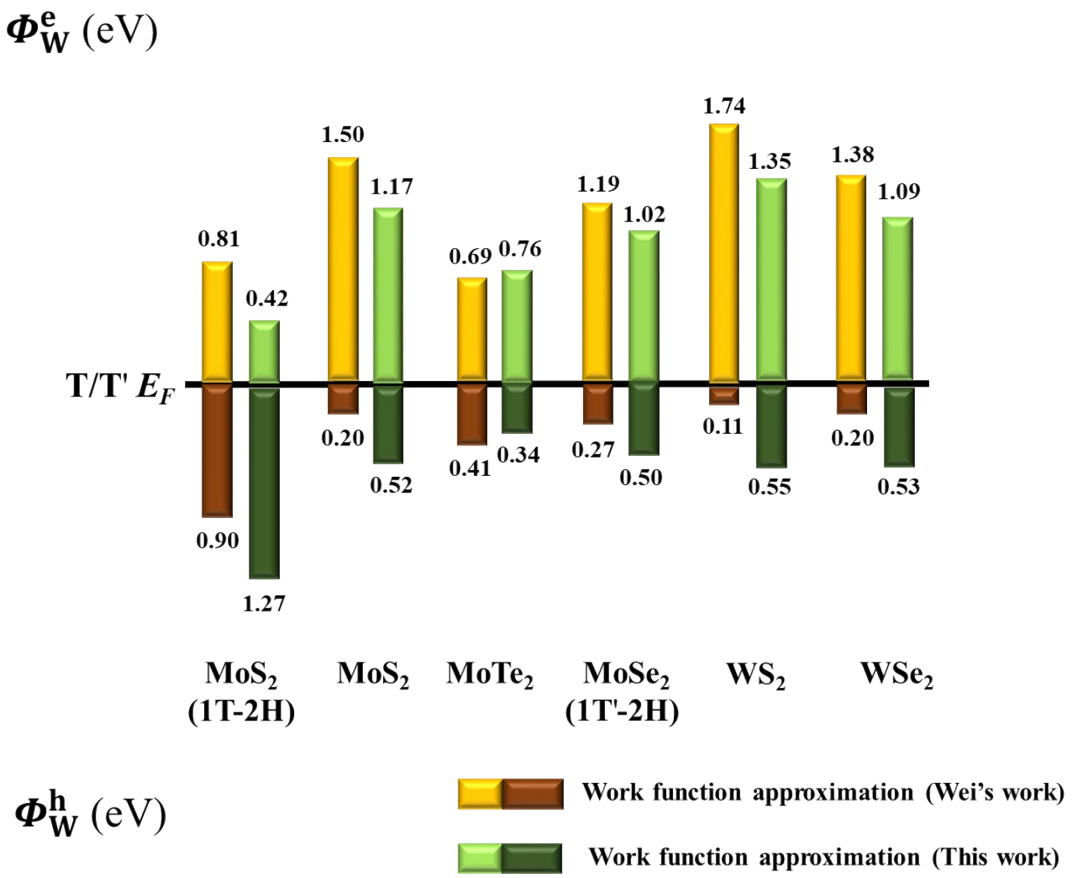

Figure S3. Comparison of the SBHs (Φ_W^e/Φ_W^h) of the work function approximation between this work and Wei's work.[1]

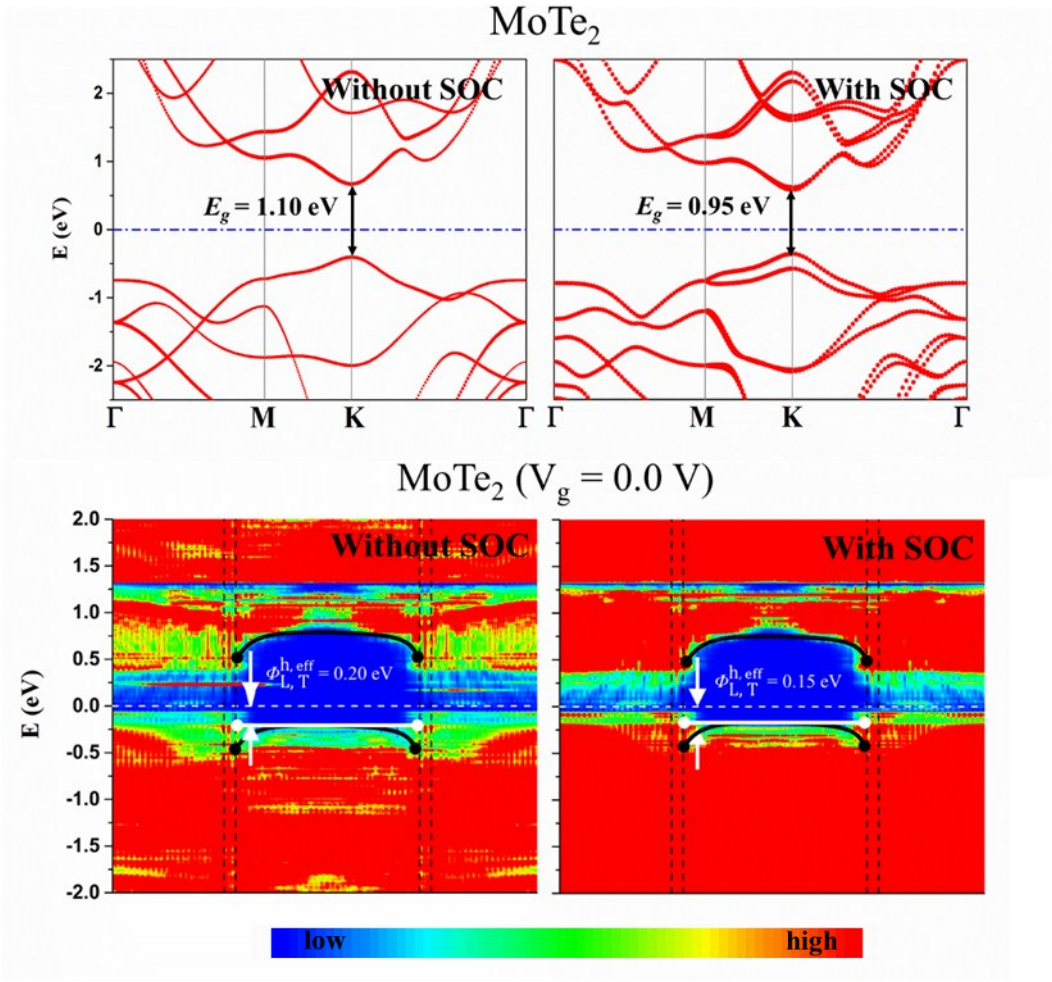

Figure S4. Comparison of the band structure and the transport SBH of the ML $MoTe_2$ 1T'-2H in-plane heterojunction without and with spin orbit coupling (SOC).

Reference

(1) Liu, Y. Y.; Stradins, P.; Wei, S. H. Van Der Waals Metal-Semiconductor Junction: Weak Fermi Level Pinning Enables Effective Tuning of Schottky Barrier. *Sci. Adv.* **2016,** *2* (4), e1600069.