Supporting information

Tuning the Electronic Properties of WS_2/Sc_2C Heterostructures via Surface Functionalization: A First-Principles Study

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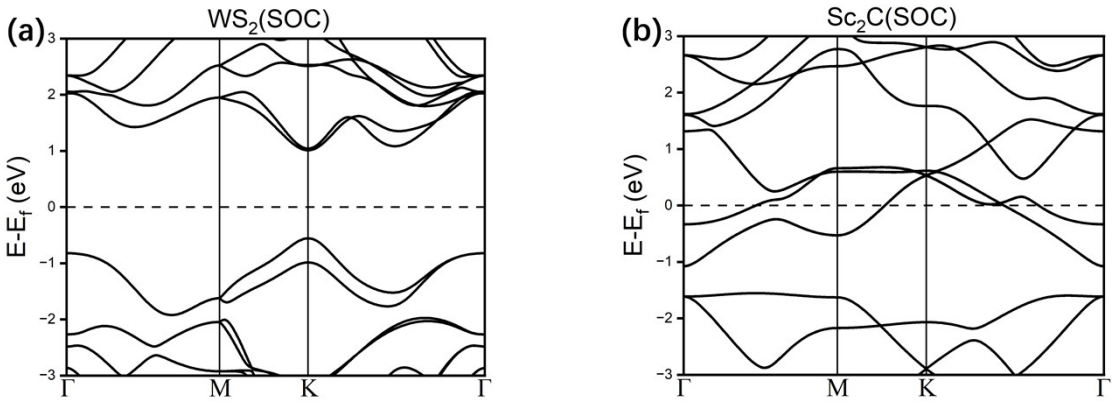

Fig. S1. Band structures of monolayer WS_2 and monolayer Sc_2C with spin-orbit coupling (SOC) considered.

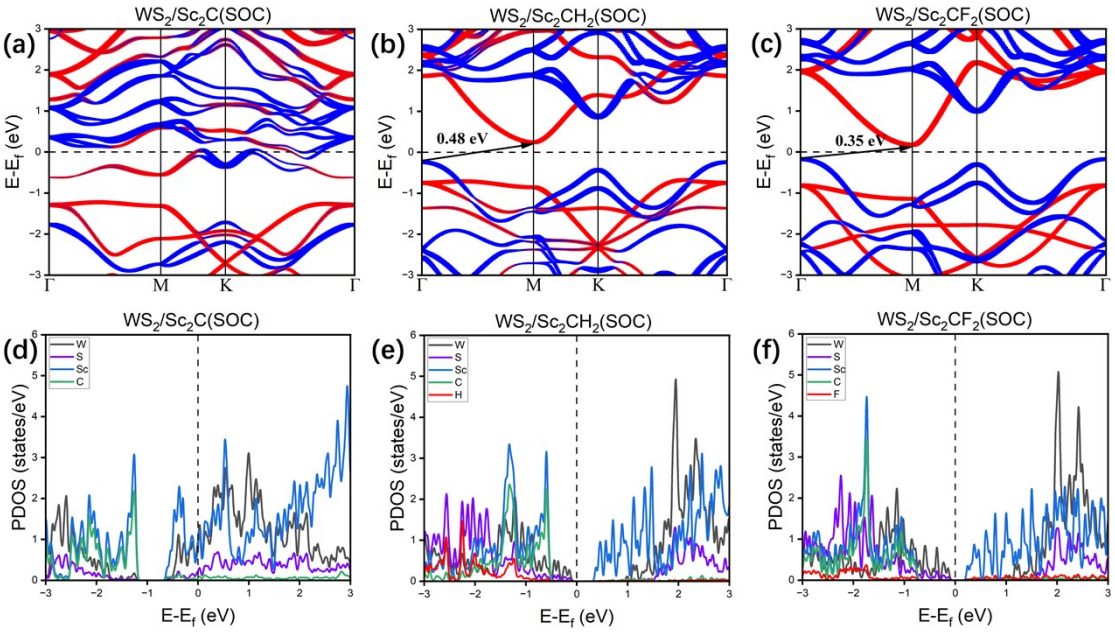

Fig. S2. Projected band structures of (a) WS_2/Sc_2C, (b) WS_2/Sc_2CH_2, and (c) WS_2/Sc_2CF_2 heterostructures with spin-orbit coupling (SOC) considered. The contributions from WS_2 and MXene are represented by the blue and red shading, respectively. The line width corresponds to the weight of the bands. Projected density of states (PDOS) of (d) WS_2/Sc_2C, (e) WS_2/Sc_2CH_2, and (f) WS_2/Sc_2CF_2 heterostructures with spin-orbit coupling (SOC) considered**.**

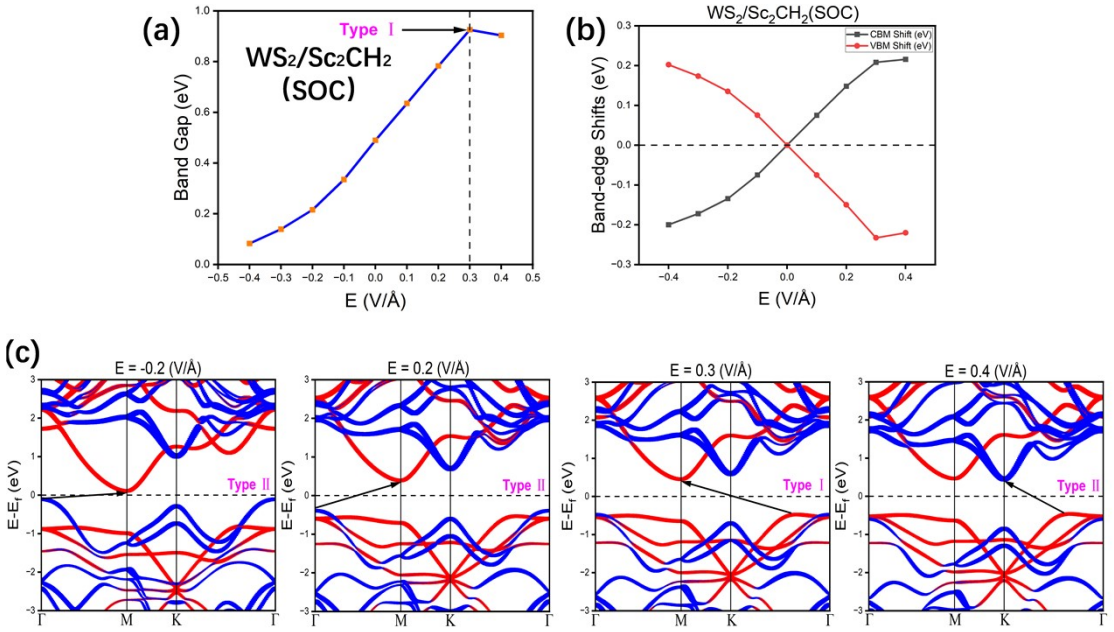

Fig. S3. (a) Variation of the band gap of the WS_2/Sc_2CH_2 heterostructure as a function of external electric field, with spin–orbit coupling (SOC) taken into account, the black arrow indicates that the heterojunction exhibits a Type I contact only at E = 0.3 V/Å. (b) Evolution of band-edge positions of the WS_2/Sc_2CH_2 heterostructure under external electric fields, considering SOC effects. (c) Projected band structures of the WS_2/Sc_2CH_2 heterostructure under various external electric fields, with SOC effects included.

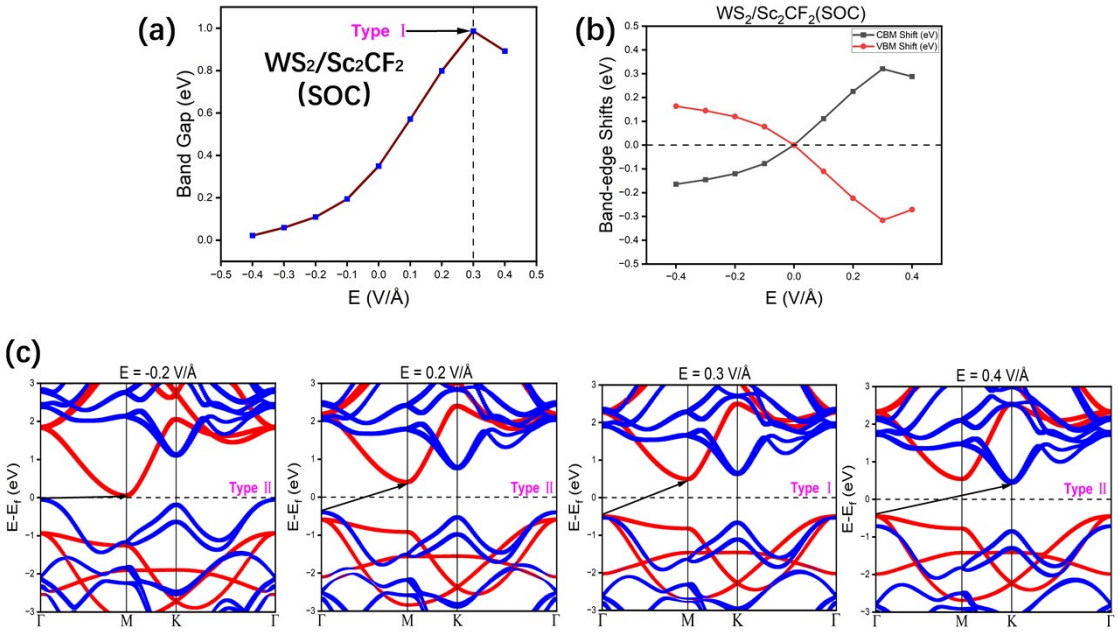

Fig. S4. (a) Variation of the band gap of the WS_2/Sc_2CF_2 heterostructure as a function of external electric field, with spin-orbit coupling (SOC) taken into account. (b) Evolution of band edge positions of the WS_2/Sc_2CF_2 heterostructure under external electric fields, considering SOC effects. (c) Projected band structures of the WS_2/Sc_2CF_2 heterostructure under various

external electric fields, with SOC effects included.

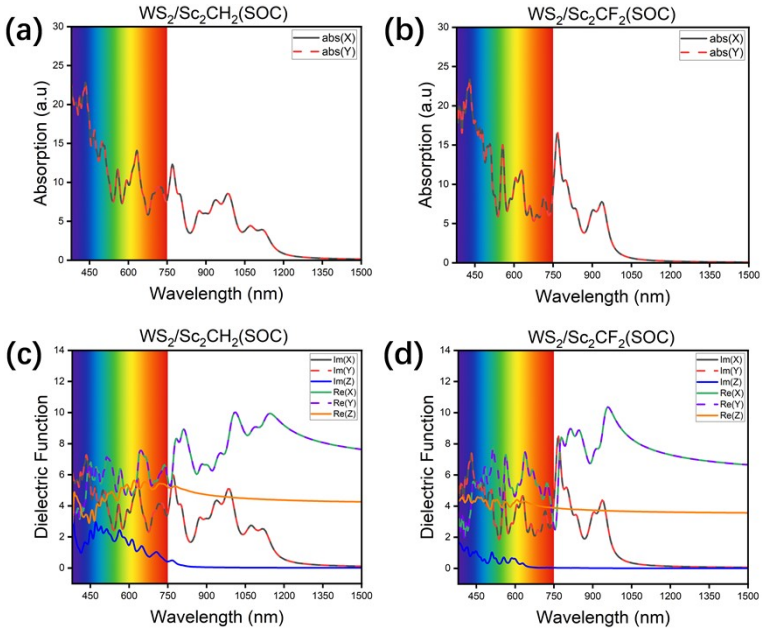

Fig. S5. Absorption spectra of (a) WS_2/Sc_2CH_2 and (b) WS_2/Sc_2CF_2 heterostructures with spin–orbit coupling (SOC) taken into account. Dielectric functions of (c) WS_2/Sc_2CH_2 and (d) WS_2/Sc_2CF_2 heterostructures with SOC effects considered.