Supplemental Material of:

P-type Ohmic contact to MoS_2 via binary compound electrodes

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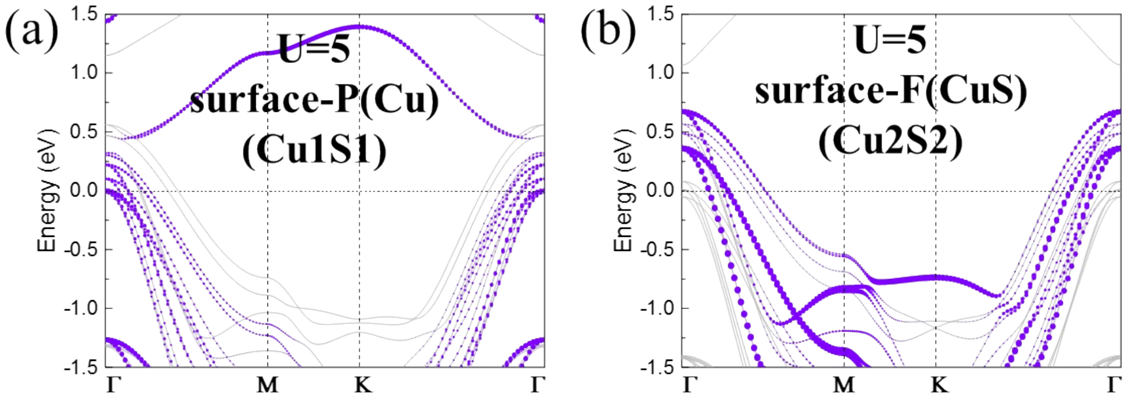

FIG. S1. The projected band structure of CuS slab with Hubbard U = 5 eV. The projected band structures of (a) P(Cu) surface (Cu1S1) and (b) F(Cu-S) surface (Cu2S2) in the CuS slab. The Fermi level was set to zero.

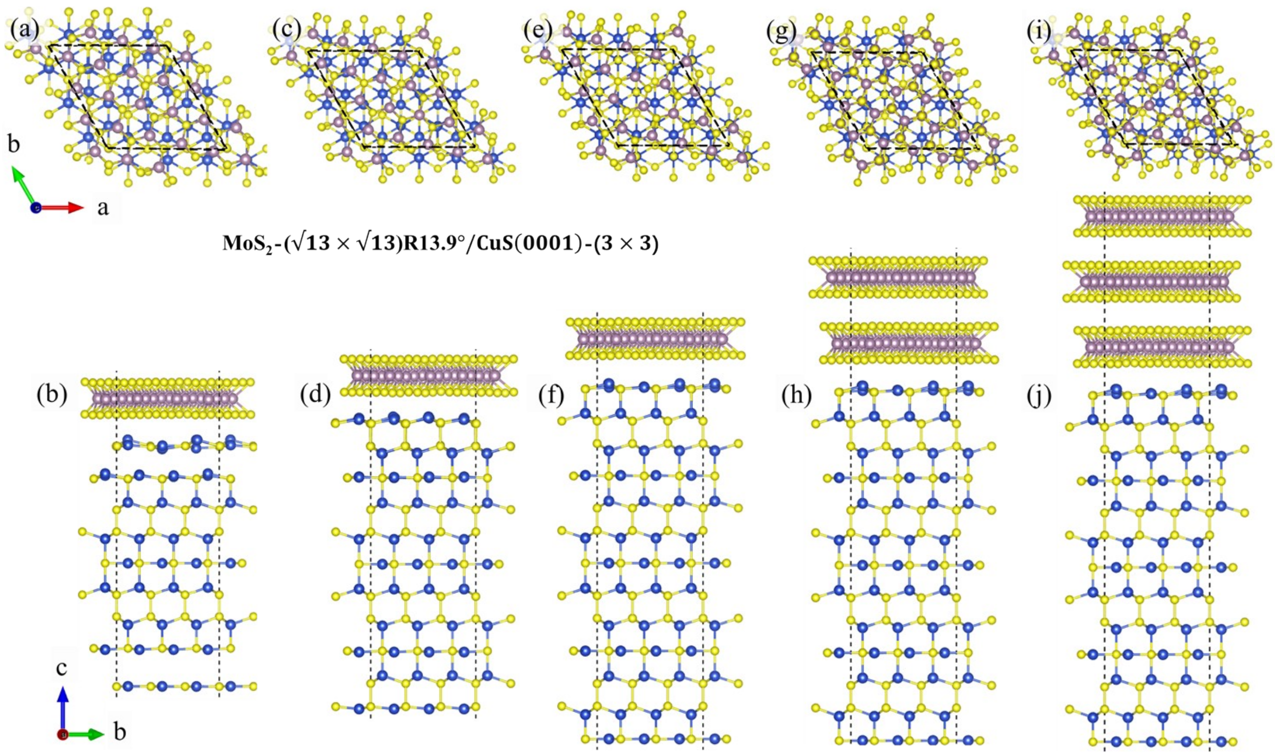

FIG. S2. The structure of CuS/MoS_2 junctions. (a) and (b) are top view and side view of P(S)/monolayer MoS_2 junction, (c) and (d) are top view and side view of P(Cu)/monolayer MoS_2 junction, (e) and (f) are top view and side view of F(Cu-S)/monolayer MoS_2 junction, (g) and (h) are top view and side view of F(Cu-S)/bilayer MoS_2 junction, and (i) and (j) are top view and side view of F(Cu-S)/trilayer MoS_2 junction, respectively. The dashed black line indicate the supercell of CuS/MoS_2 junctions.

F(Cu-S)/few-layer MoS_2 junctions. As shown in Figs. S3(a) and S3(c), the band structures of bilayer and trilayer MoS_2 with a $(\sqrt{13} \times \sqrt{13})$R13.9° supercell show an indirect band gap of 1.22 and 1.11 eV, respectively, which are in good agreement with that in the literature.[1] From monolayer to few-layer, the decrease of band gap originates from the quasi-bonding interactions between MoS_2 layers, which are significant for many layered 2D materials if the band edges of monolayer have out-of-plane orbitals that contribute to the interlayer quasi-bonding.[2-4]

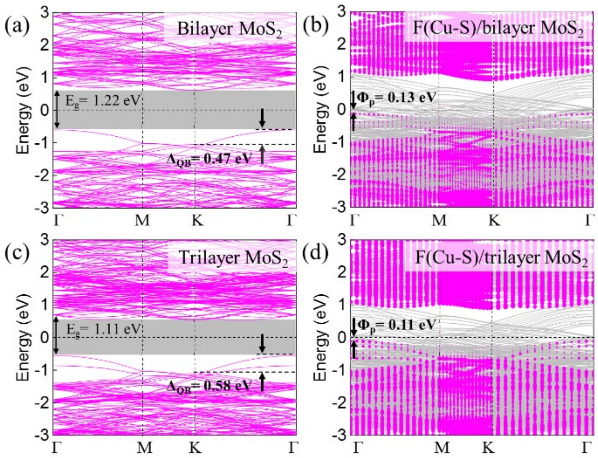

FIG. S3. Band structures of few-layer MoS_2 and the Schottky barrier heights in F(Cu-S)/few-layer MoS_2 junctions. The band structures of (a) bilayer and (c) trilayer MoS_2 with a $(\sqrt{13} \times \sqrt{13})$R13.9° supercell. The projected band structures of (b) bilayer MoS_2 in F(Cu-S)/bilayer MoS_2 junction and (d) trilayer MoS_2 in F(Cu-S)/trilayer MoS_2 junction. Φ_p represent the *p*-type SBH of holes. The Fermi level was set to zero.

Table SI. Vertical separation (D) between the outer atoms of MoS_2 and F(Cu-S) surface, work function of the F(Cu-S) surface (W_M) and the F(Cu-S) surface with MoS_2 adsorption (W_{MS}), interface potential step induced SBH correction (ΔV), QBIGS induced SBH correction (Δ_{QB}), and SBH (Φ_{SB}) in the F(Cu-S)/MoS_2 junction from the projected band structure. In the Φ_{SB} values, *p* means *p*-type Schottky barrier.

D (Å)	W_M **(eV)**	W_{MS} **(eV)**	ΔV **(eV)**	Δ_{QB} **(eV)**	Φ_{SB} **(eV)**
2.66		5.31	0.20	0.52	0.18
2.76		5.30	0.21	0.47	0.23
2.86	5.51	5.29	0.22	0.41	0.31
2.96		5.26	0.25	0.34	0.37
3.06		5.26	0.25	0.28	0.42

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