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Supporting Information

Surface Functional Groups Modification Induced Partial Fermi level Pinning and Ohmic Contact at Borophene-MoS_2 Interfaces

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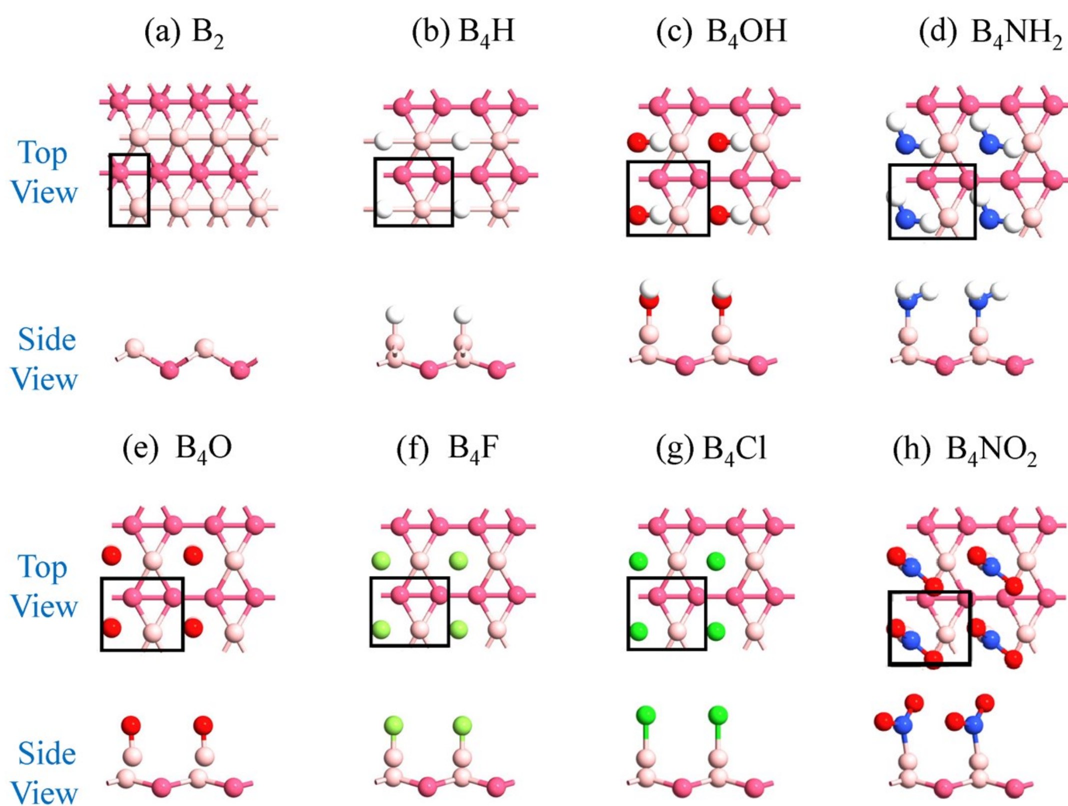

Fig. S1. Top view and side view of the most structures of monolayer (a) B_2, (b) B_4H, (c) B_4OH, (d) B_4NH_2, (e) B_4O, (f) B_4F, (g) B_4Cl, (h)B_4NO_2.

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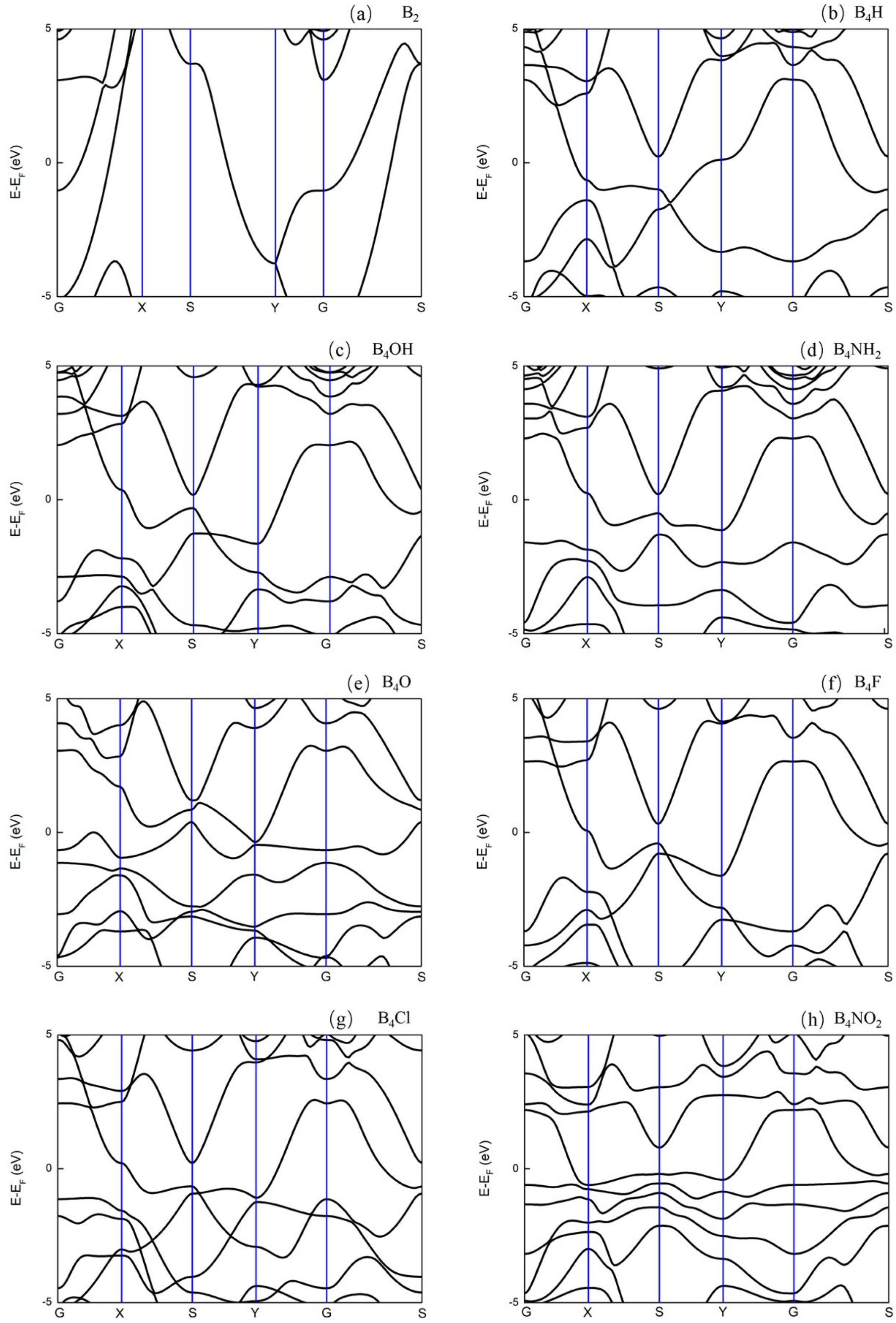

Fig. S2. Band structures of monolayer (a) B_2, (b) B_4H, (c) B_4OH, (d) B_4NH_2, (e) B_4O, (f) B_4F, (g) B_4Cl, (h)B_4NO_2.

Initial_1 Initial_2

	B_4H/MoS_2	B_4OH/MoS_2	B_4NH_2/MoS_2	B_4O/MoS_2	B_4F/MoS_2	B_4Cl/MoS_2	B_4NO_2/MoS_2
$E_{Initial_1}$ (eV)	-102.746	-118.743	-128.775	-108.843	-106.201	-101.370	-132.321
$E_{Initial_2}$ (eV)	-102.700	-118.718	-128.742	-108.847	-106.173	-101.340	-132.316

Fig. S3. Side view and the total energy of two initial stacking patterns of the B_4X/MoS_2 systems (X = H, OH, NH_2, O, F, Cl, NO_2).

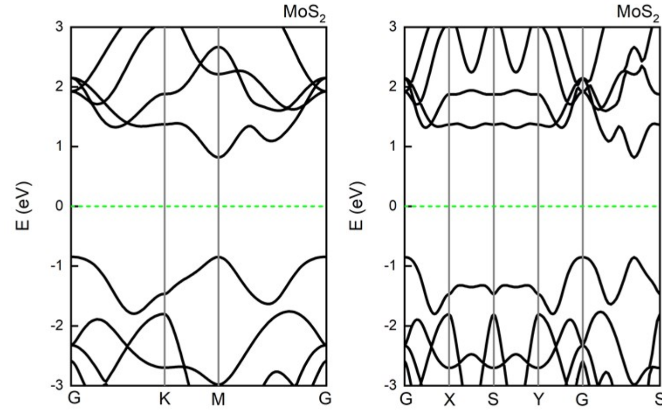

Fig. S4. Band structures of isolated ML MoS_2 in *k*-point path G→K→M→G and path G→X→S→Y→G→S.

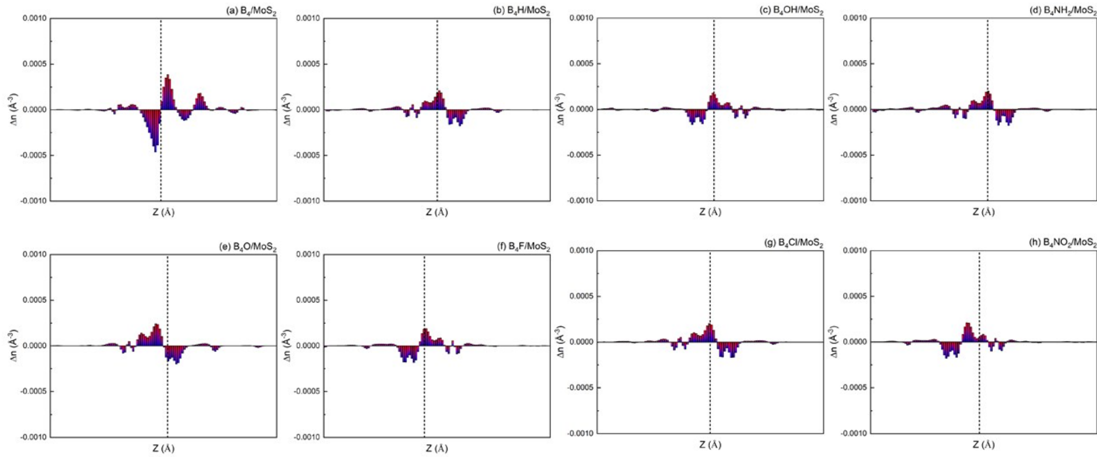

Fig. S5. Plane averaged electron density difference ($\Delta n = n_{device} - n_{electrode} - n_{channel}$) along the Z-direction of the MoS_2 transistors with different electrical contacts. Where, $n_{electrode}$, $n_{channel}$ and n_{device} are the plane-averaged electron density of isolated borophene-based metal electrode, isolated MoS_2 channel, and entire transistor device, respectively. The positive/negative values represent the charge accumulation/depletion, respectively. The dotted lines represent interfaces D.