Supporting Information

Electronic structure and interfacial contact with metallic borophene of monolayer ScSX (X=I, Br, and Cl)

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Table S1 Optimized geometric parameters of monolayer ScSX (X=I, Br, and Cl): bond lengths and bond angles.

	Sc-X (l_1,Å)	Sc-S (l_2,Å)	Sc-S (l_3,Å)	S-Sc-S (θ_1,deg)	S-Sc-X (θ_2,deg)
ScSI	2.888	2.587	2.553	85.290	95.292
ScSBr	2.665	2.582	2.558	85.252	94.910
ScSCl	2.512	2.582	2.560	85.403	94.460

Table S2 Lattice mismatch of ScSX (X=I, Br, and Cl)/borophene heterostructures.

Lattice mismatch[a]	ScSI/borophene	ScSBr/borophene	ScSCl/borophene
a direction	0.44%	-3.36%	-5.53%
b direction	0.31%	0.54%	0.71%

[a]A negative value represents the compressive strain on borophene.

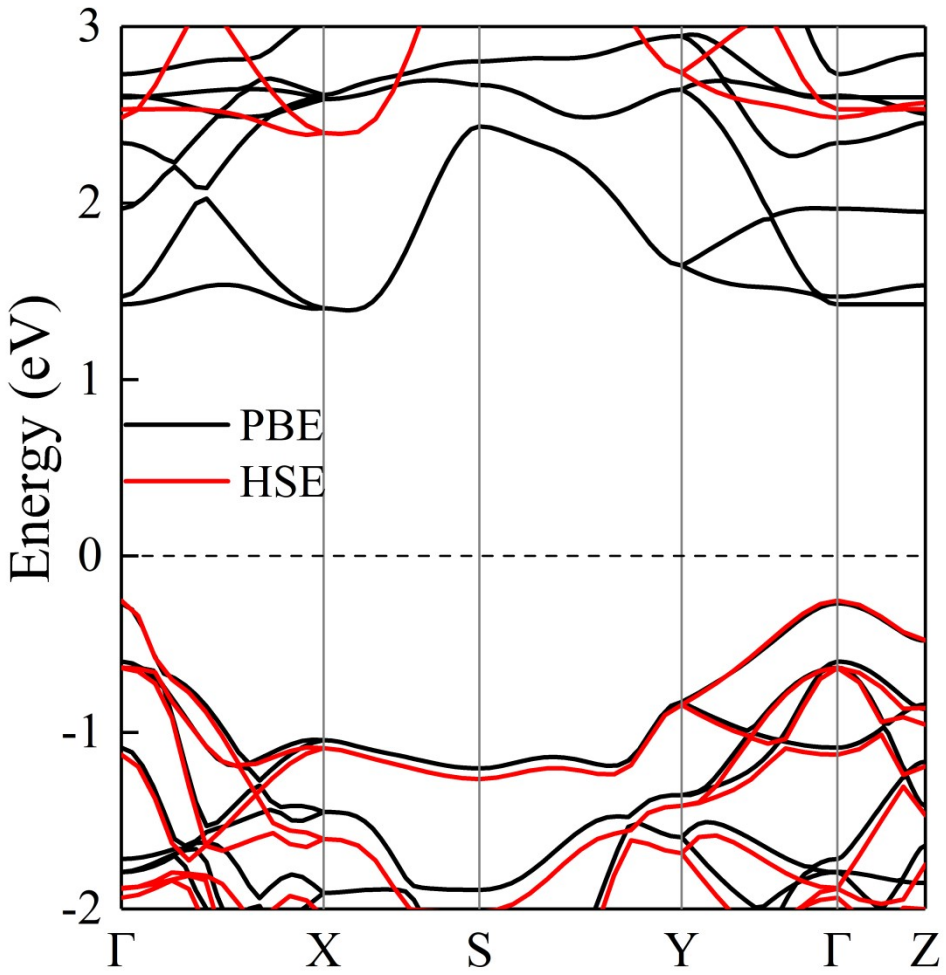

Fig. S1 Band structures of bulk ScSI with PBE and HSE06 functional.

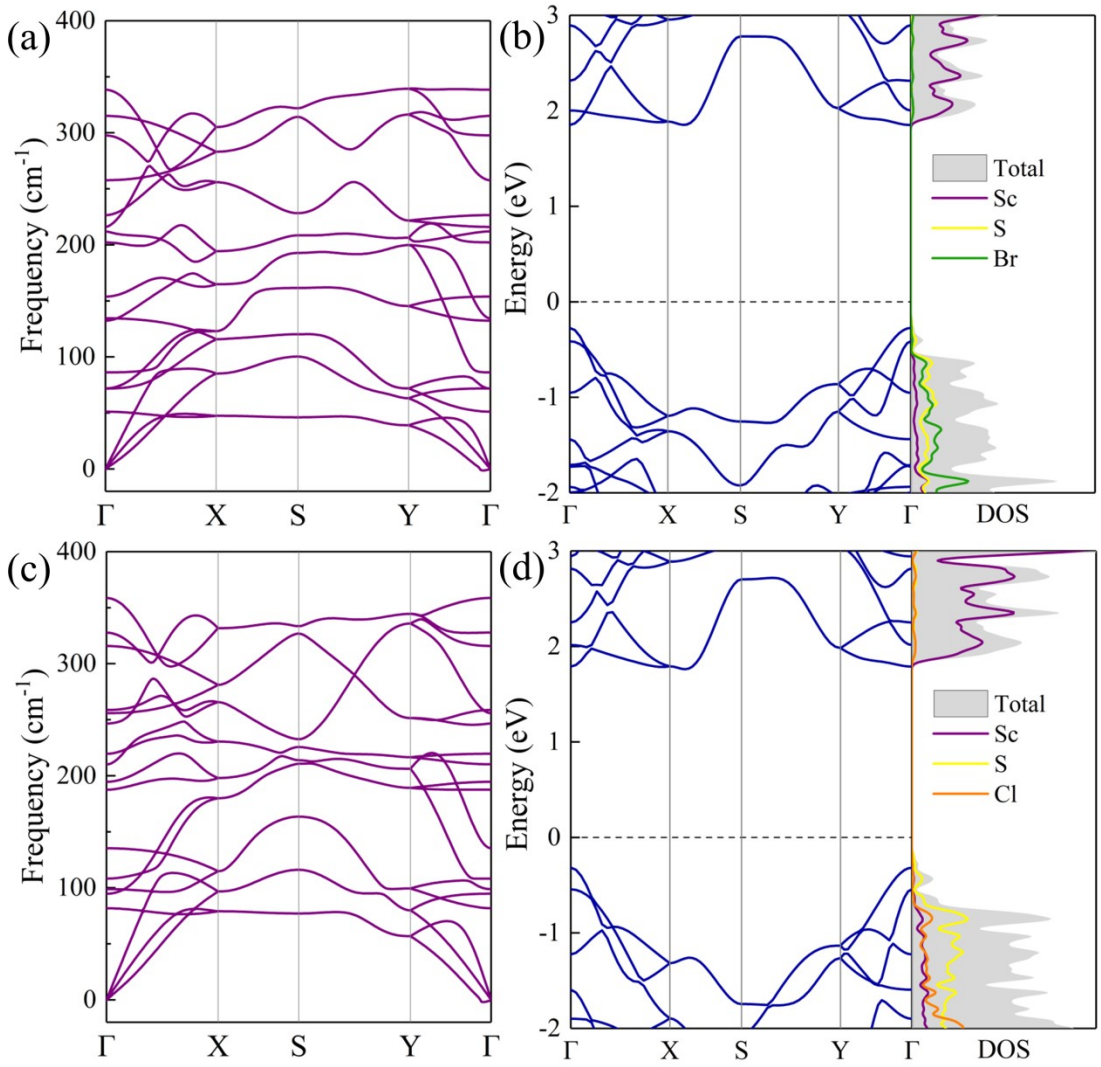

Fig. S2 (a) and (c) represent the phonon dispersion curves of monolayer ScSBr and ScSCl. (b) and (d) represent electronic band structure (left) and partial density of states (right) of monolayer ScSBr. and ScSCl.

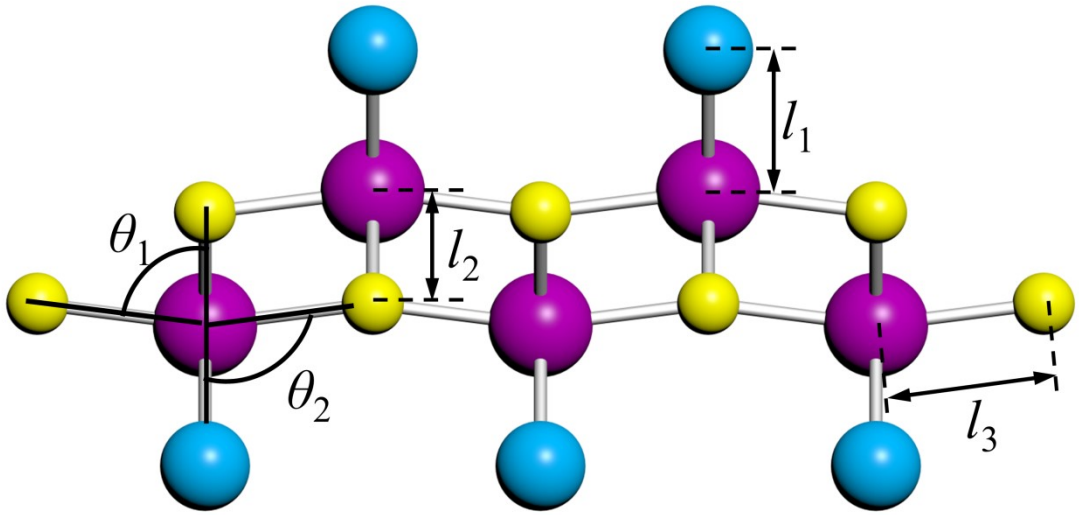

Fig. S3 Schematic diagram of bond length and bond angle of monolayer ScSI.

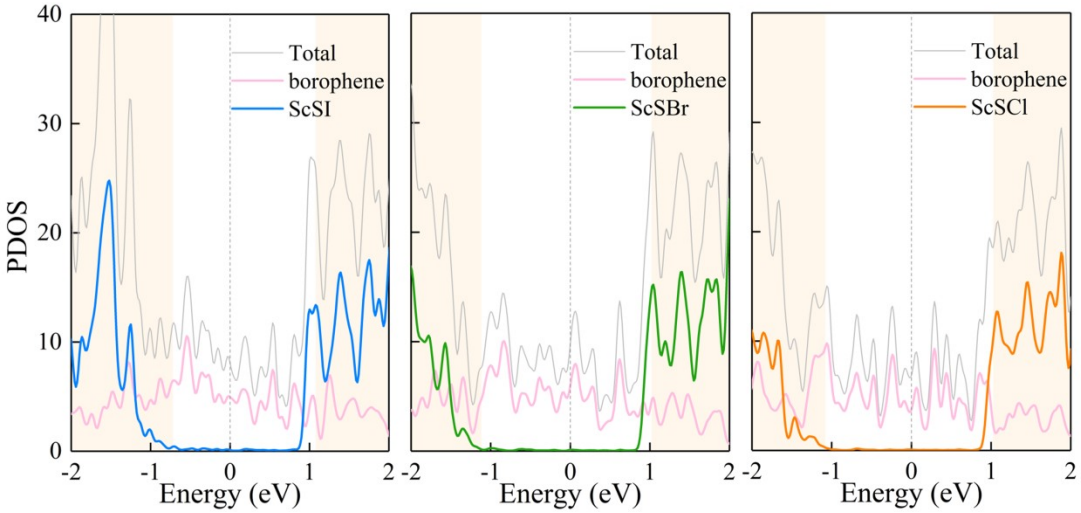

Fig. S4 Partial density of states (PDOS) of ScSX (X=I, Br, and Cl)/borophene heterostructures. The Fermi level is set to 0 eV. The orange shaded area denotes the conduction band and valence band edges of ScSX.

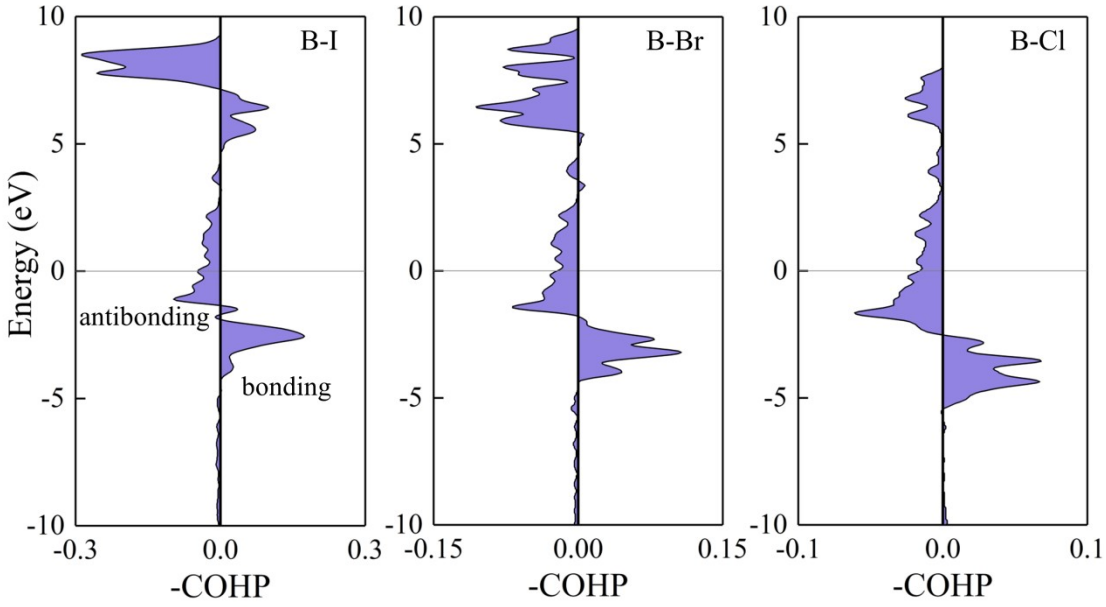

Fig. S5 The crystal orbital Hamilton population (COHP) of B-X (X=I, Br, and Cl) in ScSX/borophene heterostructures.

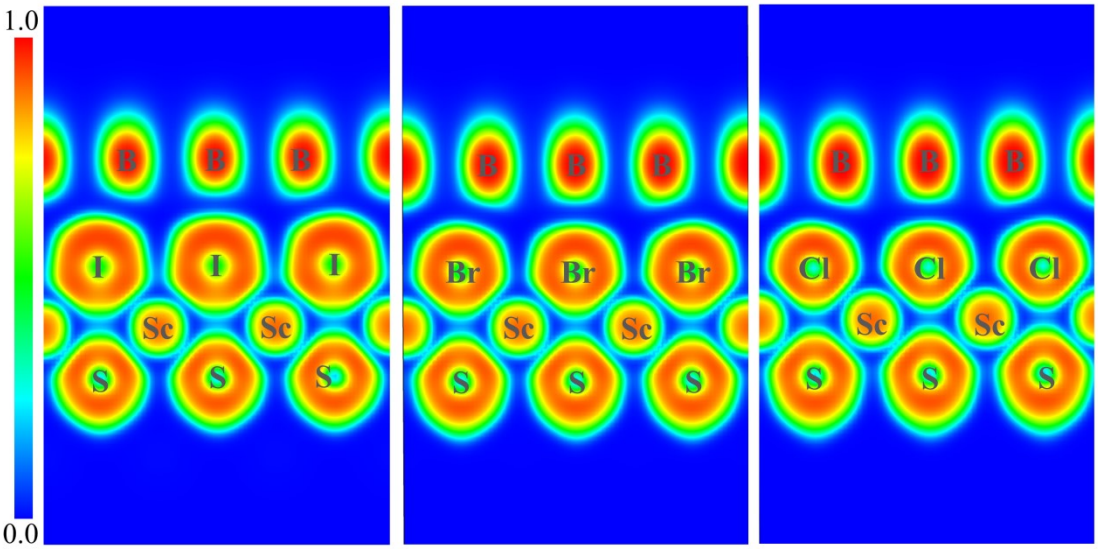

Fig. S6 The electron localization function (ELF) of ScSX (X=I, Br, and Cl)/borophene heterostructures.

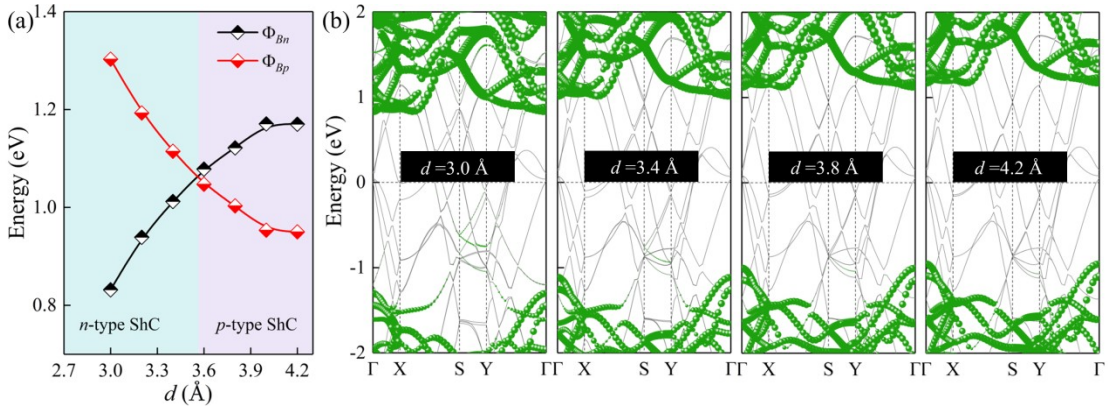

Fig. S7 (a) The change of Φ_{Bn} and Φ_{Bp}, and (b) projected band structures for ScSBr/borophene heterostructure at various interlayer spacings.

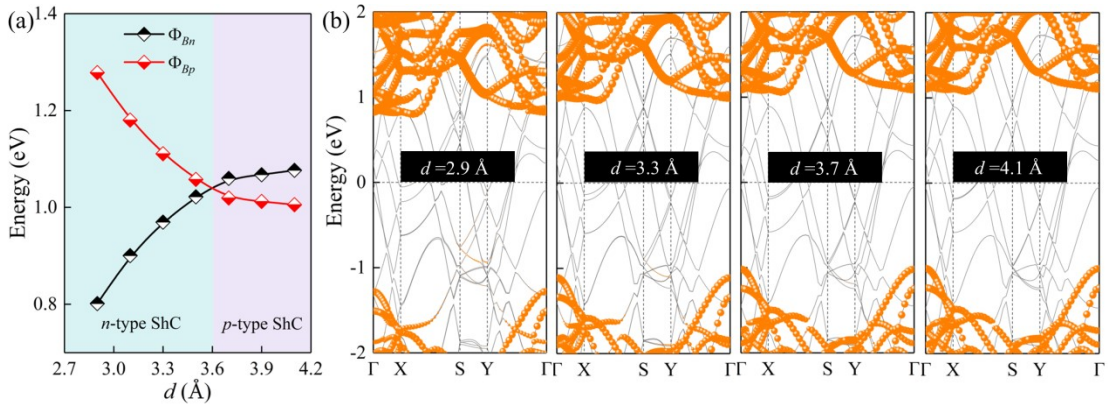

Fig. S8 (a) The change of Φ_{Bn} and Φ_{Bp}, and (b) projected band structures for ScSCl/borophene heterostructure at various interlayer spacings.

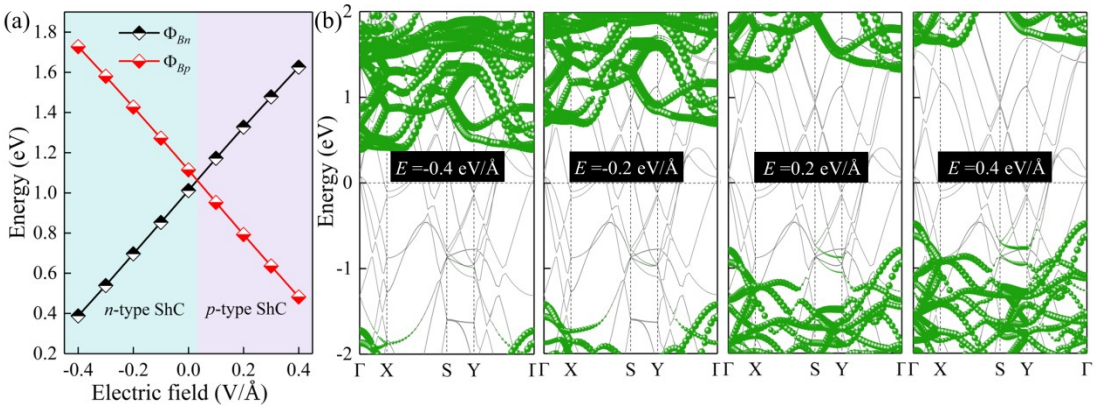

Fig. S9 (a) The change of Φ_{Bn} and Φ_{Bp}, and (b) projected band structures for ScSBr/borophene heterostructure under various external electric fields.

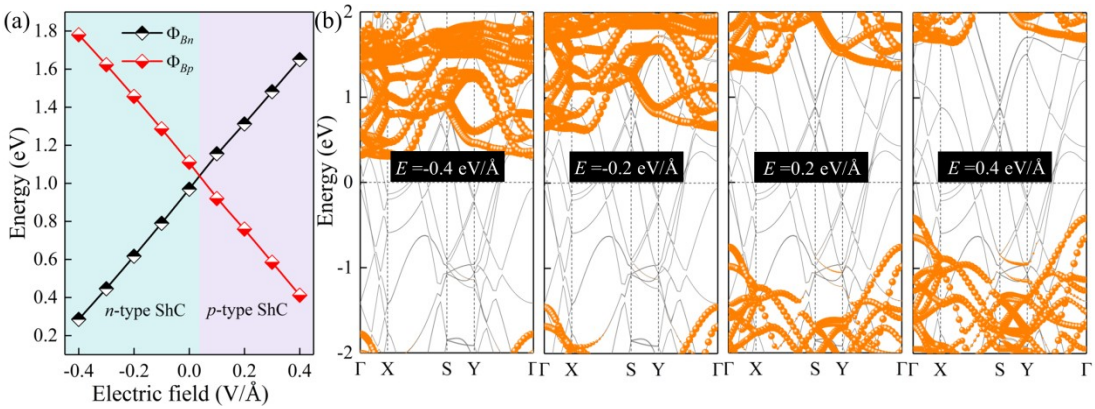

Fig. S10 (a) The change of Φ_{Bn} and Φ_{Bp}, and (b) projected band structures for ScSCl/borophene heterostructure under various external electric fields.