Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Materials

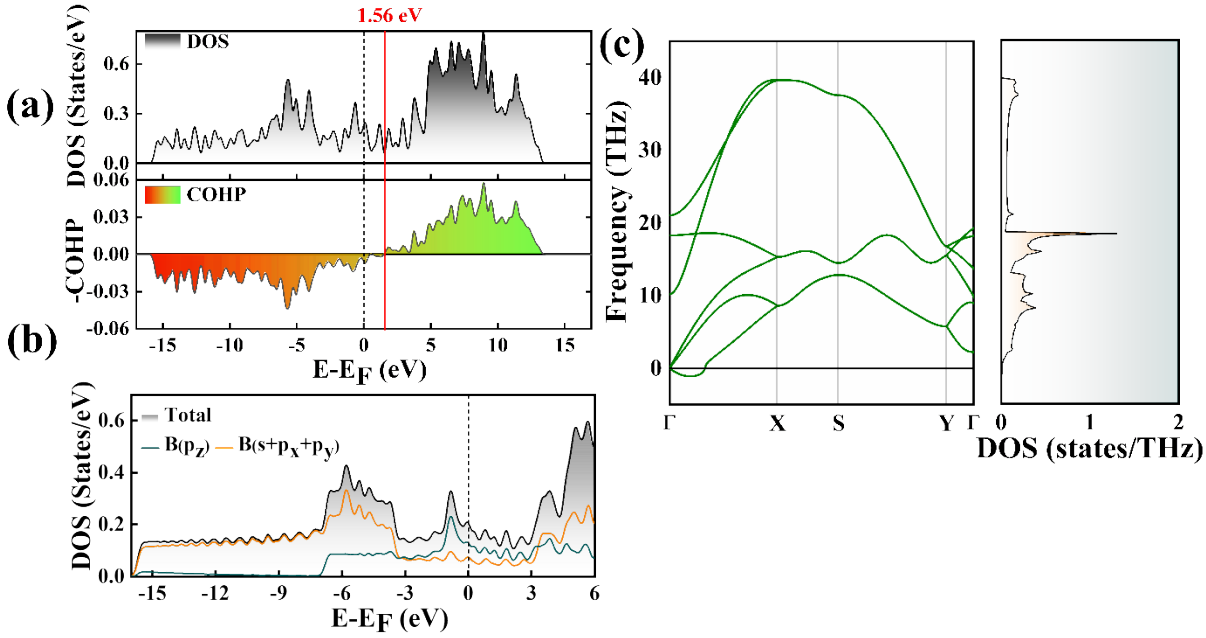

Fig. S1. ***(a)*** *COHP and total DOS curve, (b) PDOS with in-plain $s+p_x+p_y$, out of plain p_z-state of B and s-state of H atom and (c) Phonon band dispersion and phonon Density of states of 2-Pmmn Borophene.*

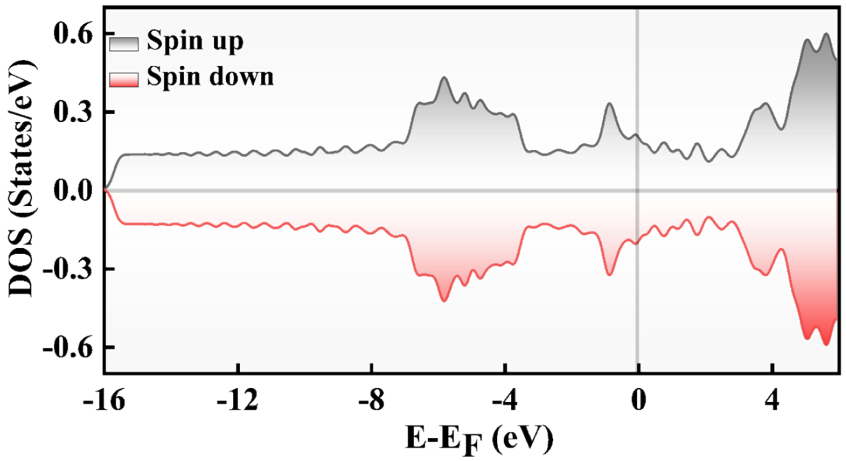

Fig. S2. *The total Density of States (DOS) of spin-up and spin-down stater of borophene*

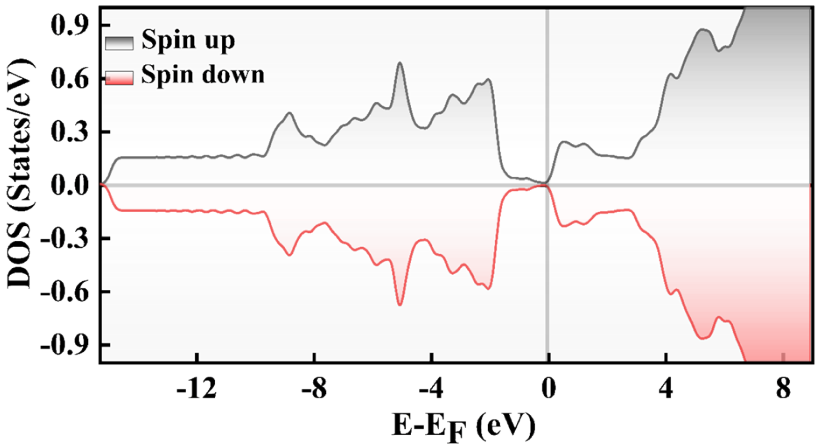

Fig. S3. *The total Density of States (DOS) of spin-up and spin-down stater of hydrogenated borophene*

Table S1. *The spin up and spin down electron contribution in* d_{xy} *and* $d_{x^2-y^2}$ *orbitals of doped atom.*

Dopant	**d_{xy} (Spin Up)**	**$d_{x^2-y^2}$ (Spin Up)**	**d_{xy} (Spin Down)**	**$d_{x^2-y^2}$ (Spin Down)**	**Spin Polarization**
V	0.9854	0.2022	0.0093	0.0699	Isotropic
Cr	0.9866	0.9281	0.0045	0.0420	Isotropic
Mn	0.9958	0.9646	0.0153	0.1345	Isotropic
Fe	0.9790	0.9391	0.9487	0.0710	Anisotropic
Co	0.9824	0.9528	0.9683	0.0964	Anisotropic
Ni	0.9795	0.9539	0.9740	0.8264	Anisotropic

Supporting Data

Table S2. *Lattice Parameters and Atomic Positions of Borophene and Hydrogenated Borophene*

Structure	Lattice Parameter	Atomic Position
Borophene	1.617975850 0.000000000 0.000000000 0.000000000 2.862297290 0.000000000	B 0.4044939630 0.7155743232 12.5488840239
2-Pmmn	0.000000000 0.000000000 25.992524132	B 1.2134818879 2.1467229686 13.4434711783
Hydrogenated	1.945126968 0.000000000 0.000000000 0.000000000 2.813012944 0.000000000	B 0.4862593083 0.7032523303 12.5921950618
Borophene	0.000000000 0.000000000 25.992524132	H 0.4862598600 0.7032523303 11.4122231213
		B 1.4588226403 2.1097569900 13.4001603047
		H 1.4588238566 2.1097569900 14.5801319166