Supporting information

A Theoretical Insight into a Feasible Strategy of Fabrication of Borophane

Gangqiang Qin, Aijun Du and Qiao Sun

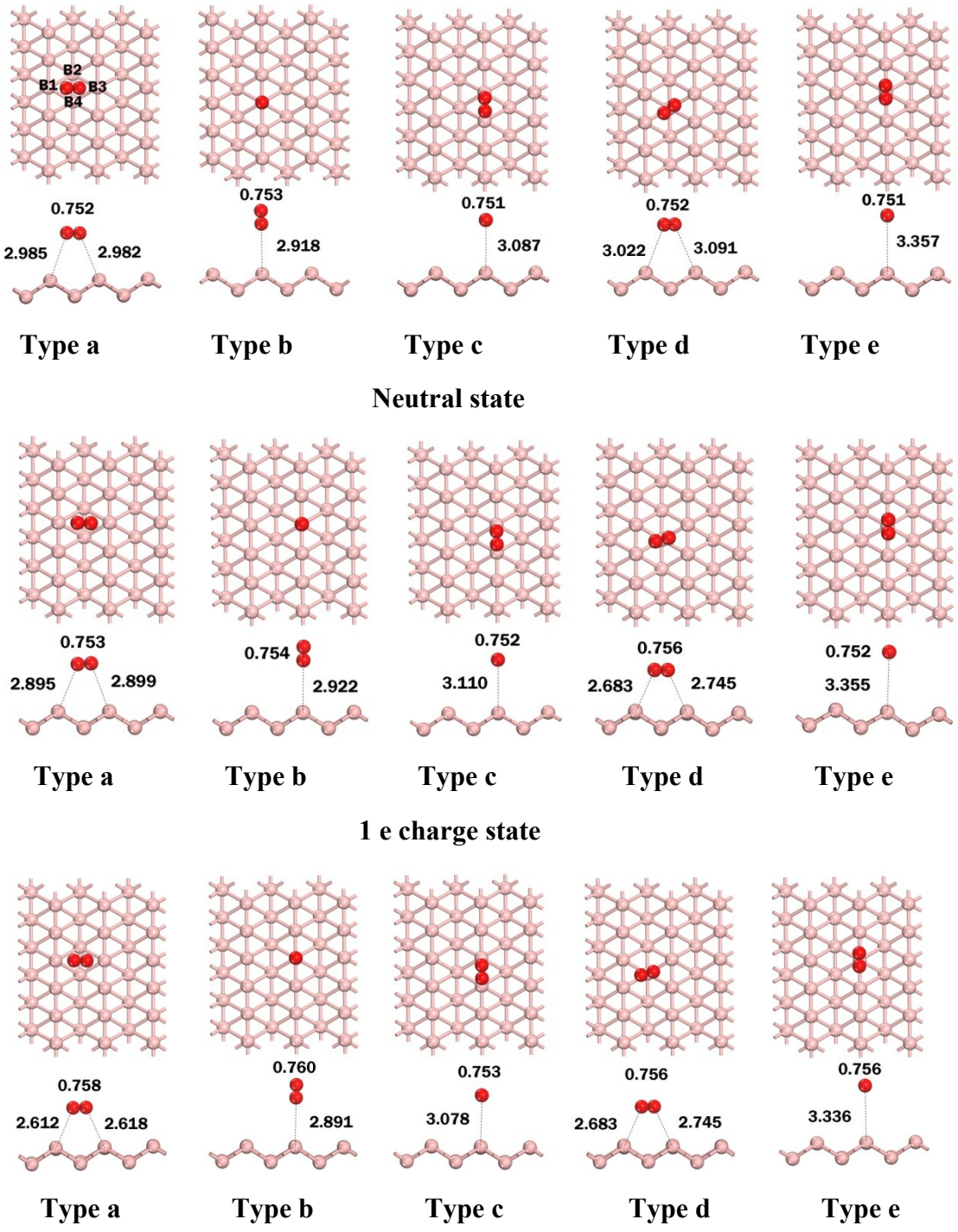


Fig. S1 Top and side views of H_2 interacting with borophene in five types of adsorption sites with different charge states.

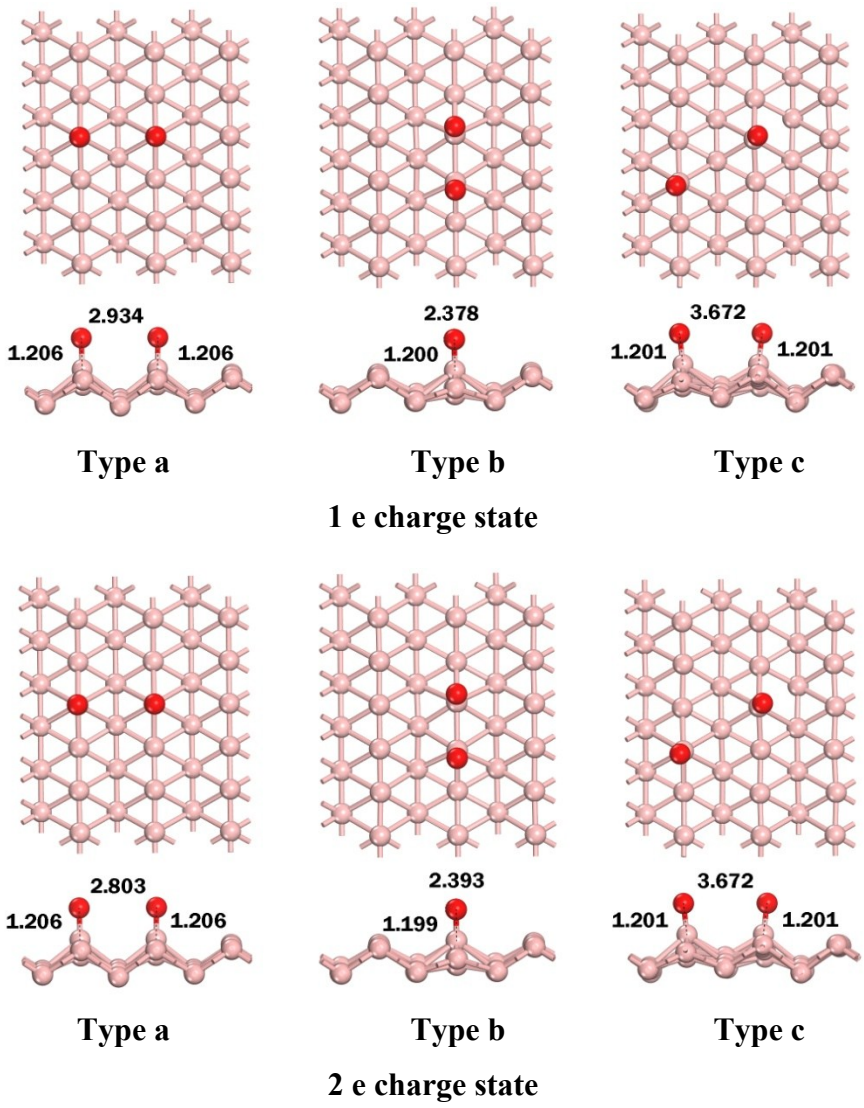


Fig. S2 Top and side views of H_2 dissociation on borophene with different charge states.

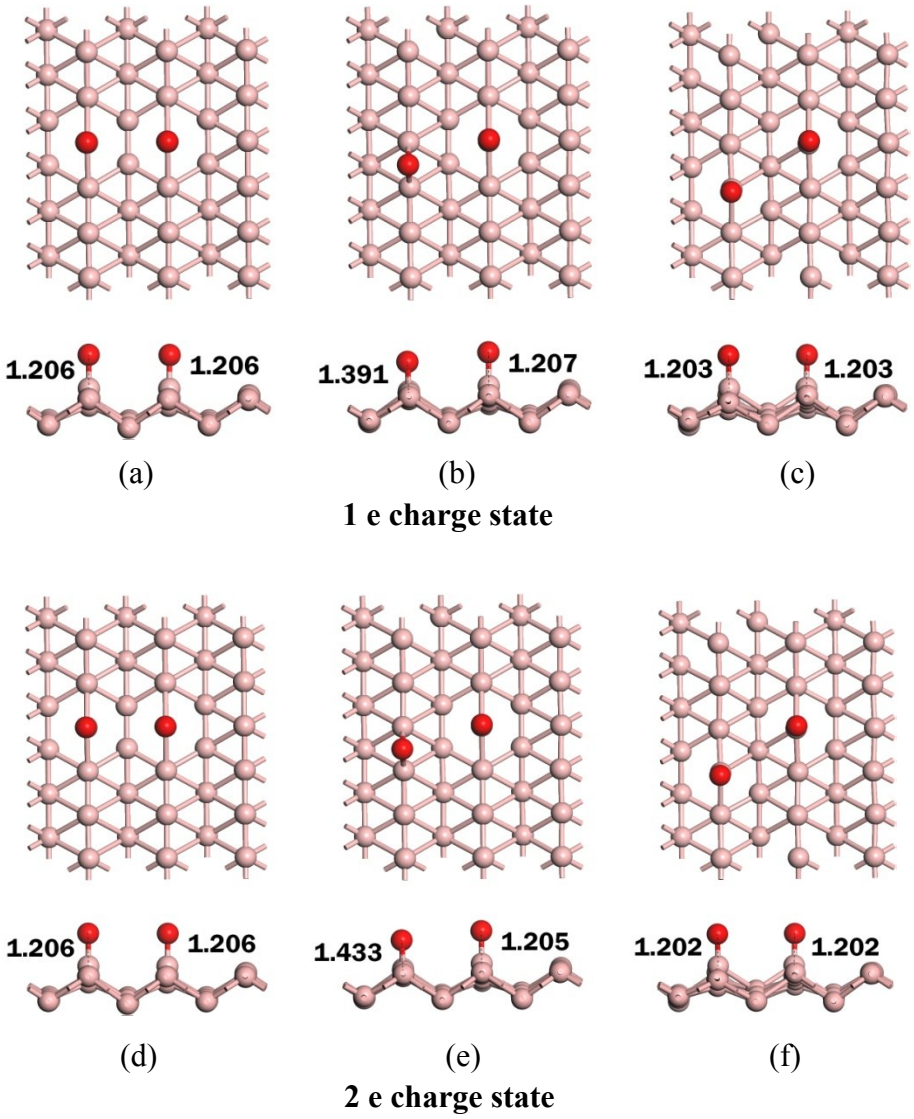


Fig. S3 Top and side views of (a) IS1, (d) IS2, (b)TS1, (e)TS2, (c) FS1, (f) FS2 of H diffusion on borophene, the indices 1 and 2 refer to the surfaces with +1 e and + 2 e charges per 6 × 3 unit cell.

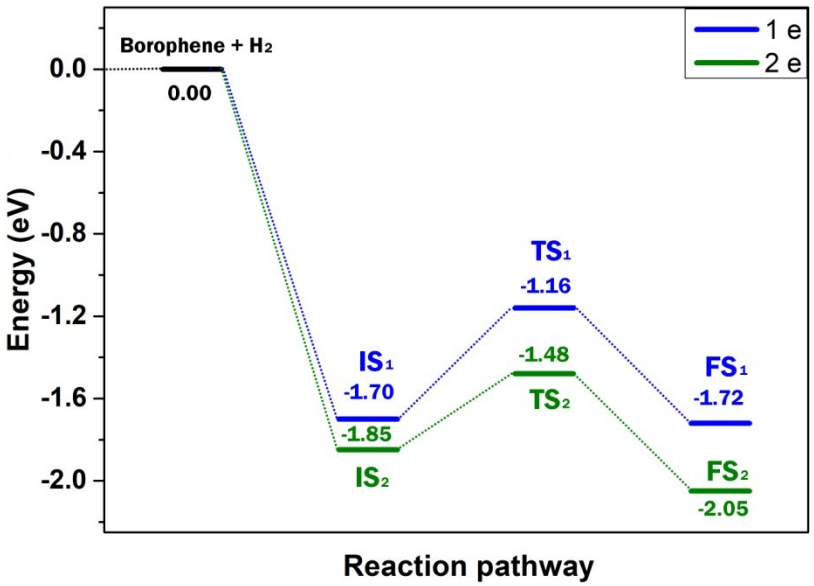
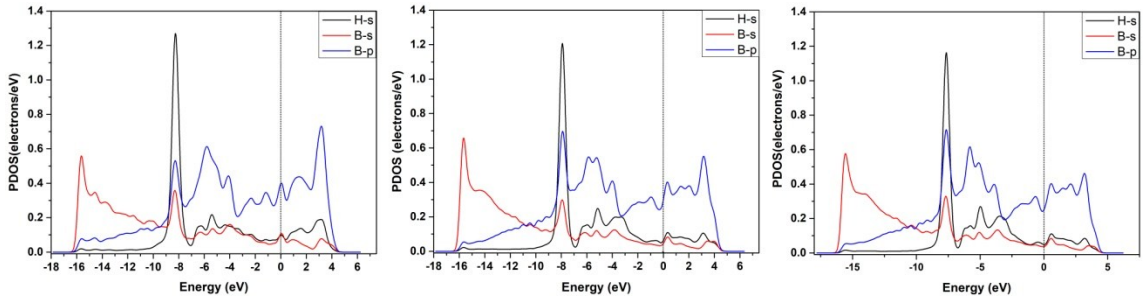


Fig. S4 Energy profiles of H diffusion on borophene with 1 e and 2 e charge state.



(a) (b) (c)

Fig. S5 The PDOS of B1 and H atoms of TS structures with the neutral (a), 1e (b) and 2e (c) charge state, respectively.

Table S1. The essential properties (H-H bond length, distance between borophene and H_2 molecule, charge transfer from borophene to H_2 molecule, and adsorption energy) of H_2 adsorption on borophene in different sites with different charge states.

Adsorption	Bond length H-H(Å)	Distance B...H (Å)	Charge transfer (e)	Adsorption energy(eV)
Neutral state				
Type a	0.752	2.982	0.002	-0.064
Type b	0.753	2.918	-0.010	-0.059
Type c	0.751	3.087	0.004	-0.036
Type d	0.752	3.022	0.005	-0.060
Type e	0.751	3.357	0.000	-0.044
1 e				
Type a	0.753	2.895	0.025	-0.099
Type b	0.754	2.922	0.000	-0.085
Type c	0.752	3.110	0.016	-0.072
Type d	0.756	2.683	0.022	-0.096
Type e	0.752	3.355	0.007	-0.075
2e				
Type a	0.758	2.612	0.081	-0.209
Type b	0.760	2.891	0.014	-0.205
Type c	0.753	3.078	0.038	-0.181
Type d	0.756	2.683	0.081	-0.206
Type e	0.756	3.336	0.019	-0.179

Table S2. The essential properties (distance between two dissociated H atoms, distance between B and H atom, charge transfer from borophene to two H atoms, and reaction energy) of H_2 dissociated on borophene in different sites with different charge states.

	Distance H...H(Å)	Distance B...H (Å)	Charge transfer (e)	reaction energy (eV)
Neutral state				
Type a	2.990	1.206	0.072	1.509
Type b	2.378	1.200	0.184	0.836
Type c	3.672	1.201	0.284	1.370
1 e				
Type a	2.934	1.206	0.102	1.694
Type b	2.378	1.200	0.164	1.187
Type c	3.672	1.201	0.262	1.708
2e				
Type a	2.803	1.206	0.074	1.847
Type b	2.393	1.199	0.182	1.708
Type c	3.672	1.201	0.263	1.847

Table S3. The atomic charge distributions of B1-B4 atoms and H_2 molecule with different charge states.

	0 e	1 e	2 e
B1	0.014	0.031	0.040
B2	-0.001	0.030	0.073
B3	0.015	0.032	0.040
B4	0.000	0.032	0.074
H_2	0.002	0.025	0.081