Supporting Information for
Structures, Mechanics and Electronics of Borophanes

Maolin Yu, Zhuhua Zhang* and Wanlin Guo

Key Laboratory for Intelligent Nano Materials and Devices of Ministry of Education, State Key Laboratory of Mechanics and Control of Mechanical Structures, Institute for Frontier Science of Nanjing University of Aeronautics and Astronautics, Nanjing 210016, China.

*E-mail: chuwazhang@nuaa.edu.cn

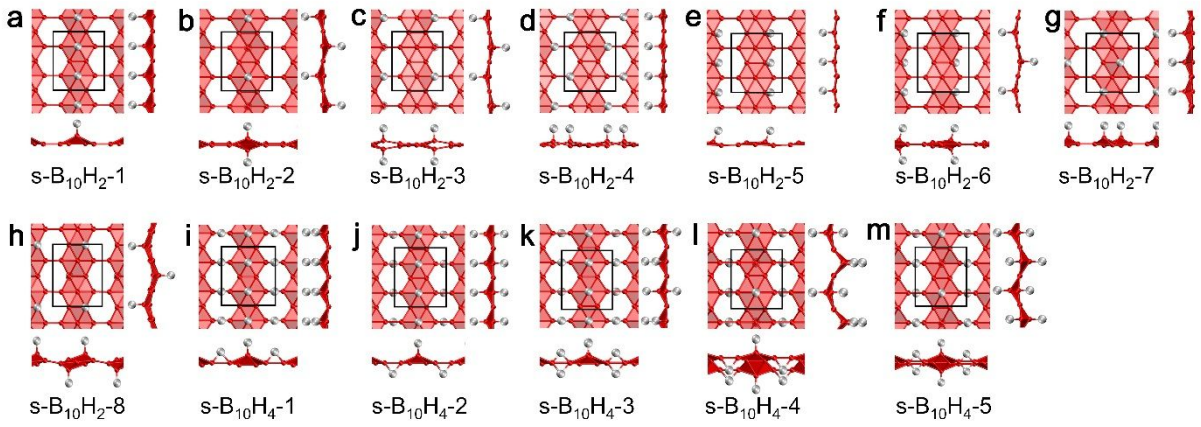

Figure S1. 13 additional borophane structures made from two combination modes mentioned in the main text. The red and sliver balls denote the B and H atoms, respectively.

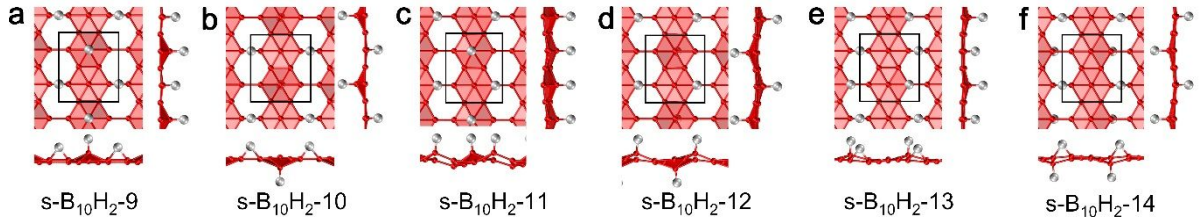

Figure S2. 6 borophane structures with hydrogen adsorbed alternately on the four sites along the FH rows. The red and sliver balls denote the B and H atoms, respectively.

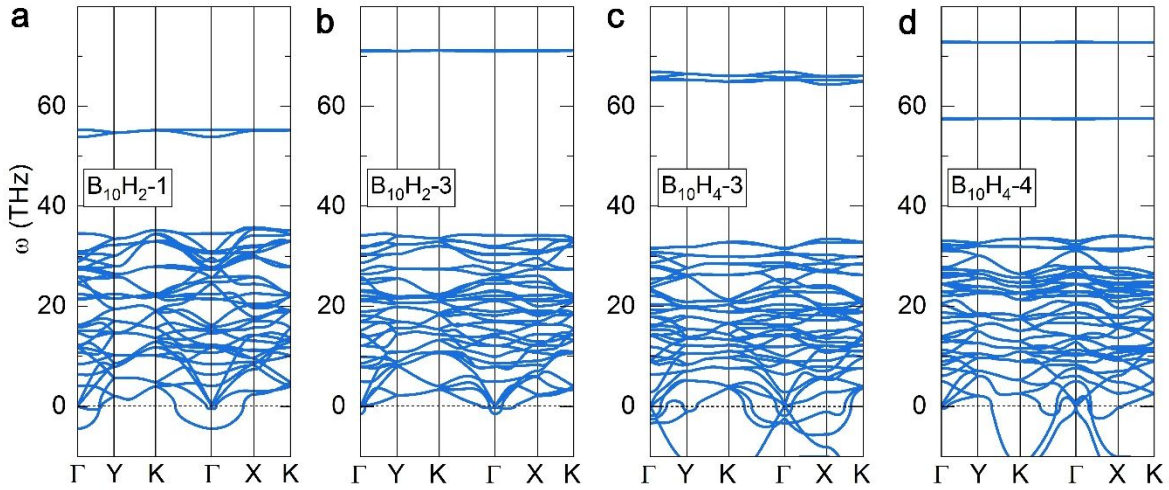

Figure S3. Phonon spectra of (a) $B_{10}H_2$-1, (b) $B_{10}H_2$-3, (c) $B_{10}H_4$-3 and (d) $B_{10}H_4$-4 structures.

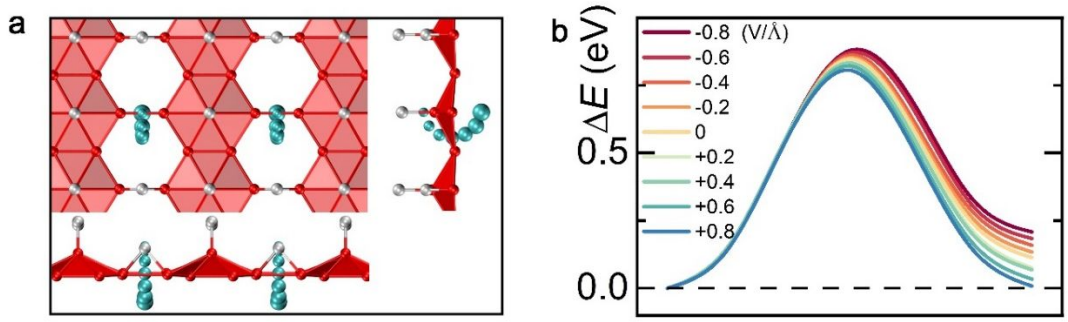

Figure S4. (a) Schematic progress of the flipping of H atoms across the boron sheet. (b) Variation of barriers for the flipping of H atoms as a function of the external electric fields. The electric fields are positive along the +z direction.

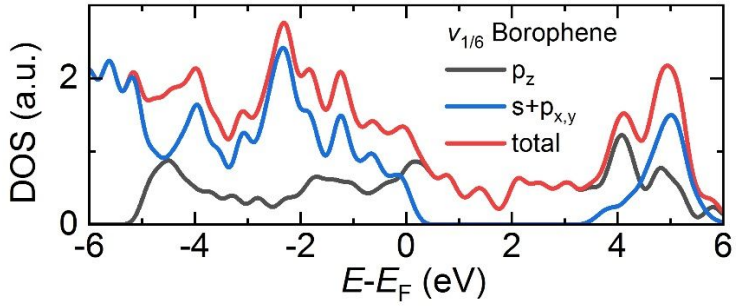

Figure S5. Calculated partial density of states (PDOS) for the pristine $v_{1/6}$ boron sheet. The in-plane bonding σ and antibonding σ^* states can be clearly identified by the blue lines.

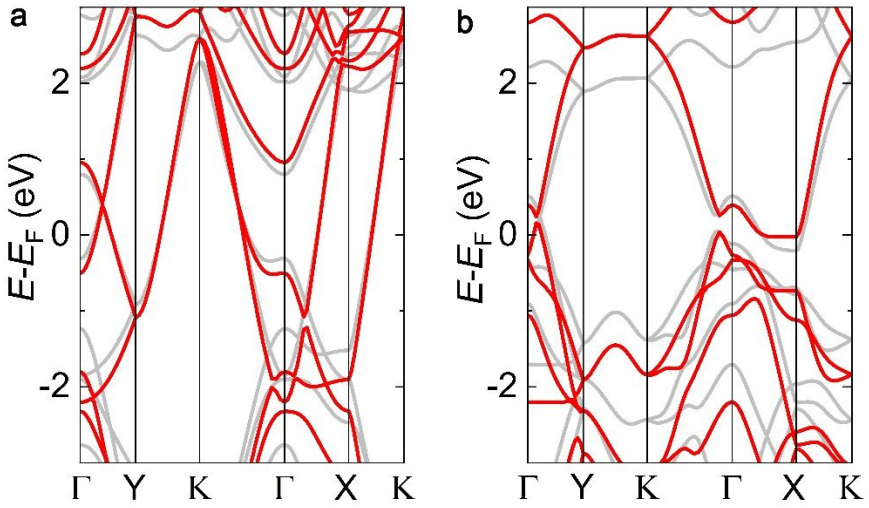

Figure S6. Calculated band structures of (a) $B_{10}H_4$-1 and (b) $B_{10}H_2$-4 by the HSE06 functional. Red and grey lines are from HSE06 and PBE functionals, respectively.

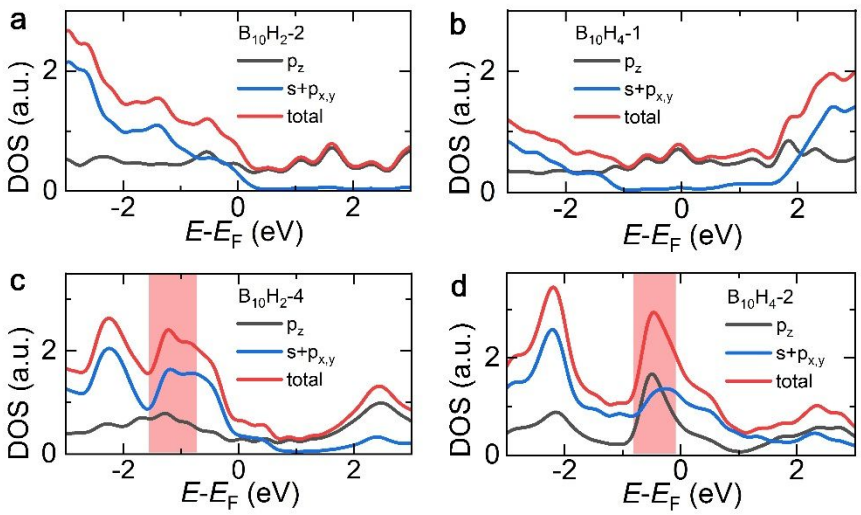

Figure S7. Calculated PDOS for (a) $B_{10}H_2$-2, (b) $B_{10}H_4$-1, (c) $B_{10}H_2$-4, and (d) $B_{10}H_4$-2 structures. The DOS peaks formed in the $B_{10}H_2$-4 and $B_{10}H_4$-2 are marked in red.

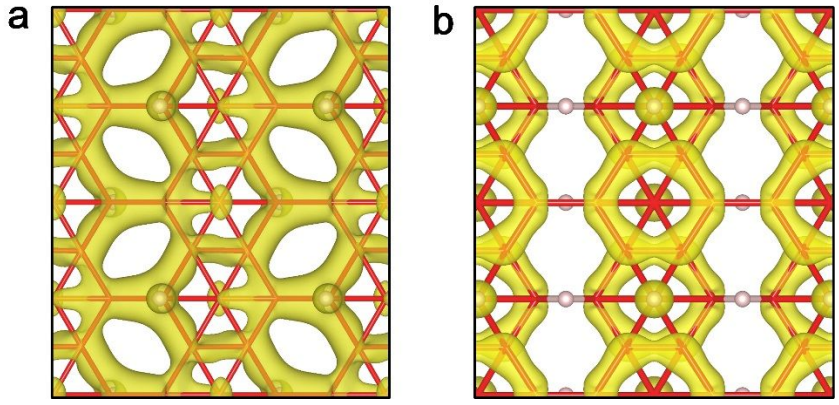

Figure S8. Isosurface plots (0.03 e/Å) of the partial charge density corresponding to the DOS peaks for (a) $B_{10}H_2$-4 at an energy window of [-1.3, -1.0 eV] and (b) $B_{10}H_4$-2 at an energy window of [-0.55, -0.25 eV] below the Fermi level.