Supporting information

Two-dimensional honeycomb borophene oxide: Strong anisotropy and nodal loop transformation

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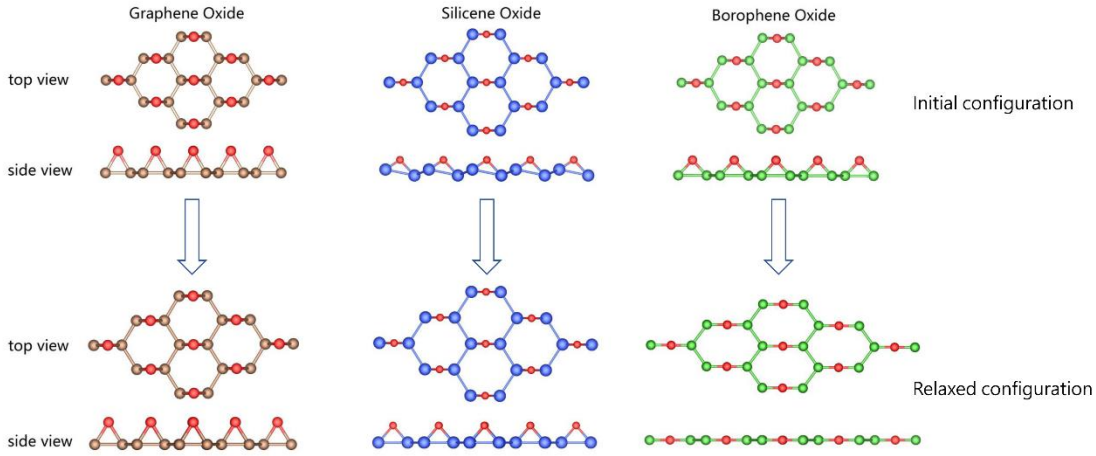

Figure S1. The oxide configurations for graphene, silicene and borophene. Previous experiment on black phosphorene has demonstrated that the oxidation process can be well-controlled through the assistance of Laser[1]. The similar technique may also be applied here for realizing h-B_2O.

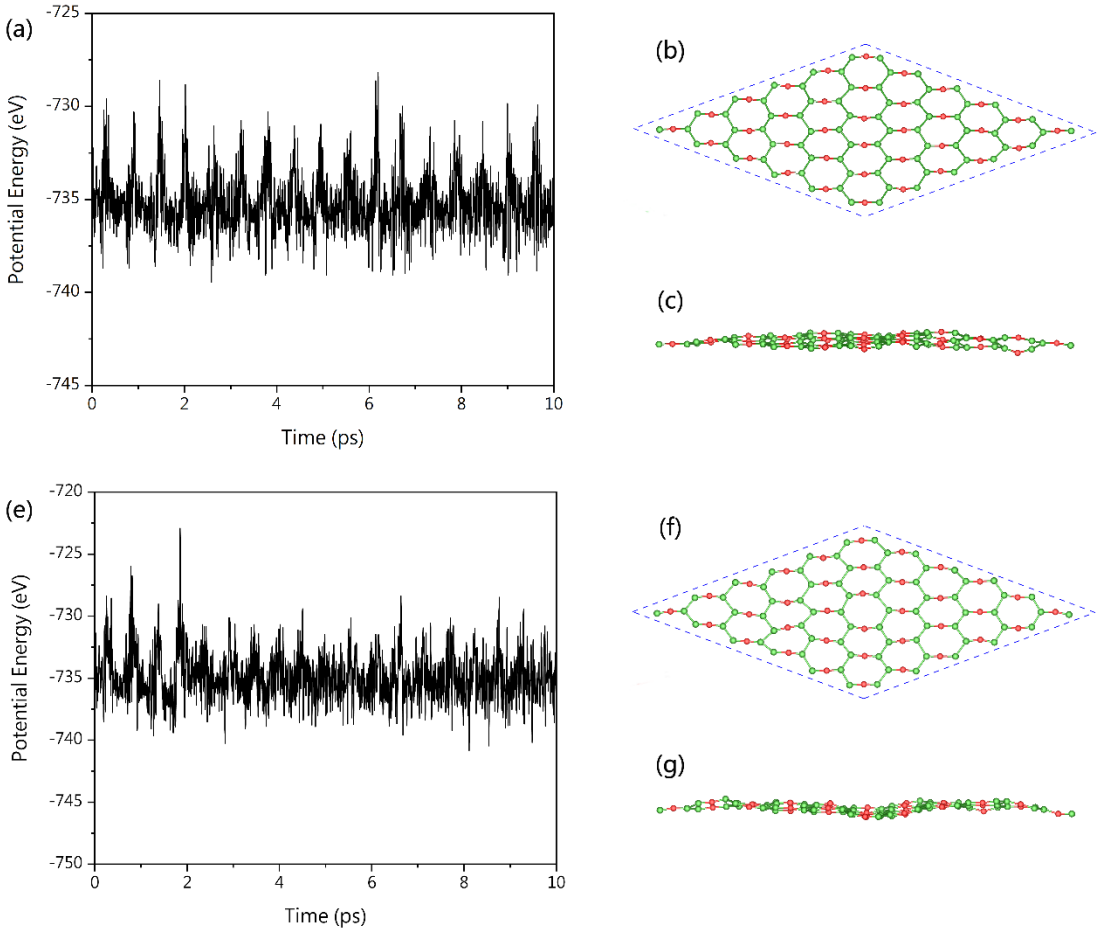

Figure S2. (a/e) The total potential energy fluctuation of h-B_2O during AIMD simulation at 800k and 1000k, respectively. (b)(c)/(f)(g) The atomic configuration of h-B_2O after 10 ps of AIMD simulation at 800k and 1000k, respectively.

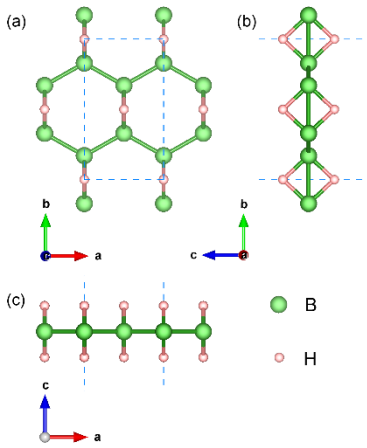

Figure S3. The top view (a) and side view (b, c) of h-B_2H_2.

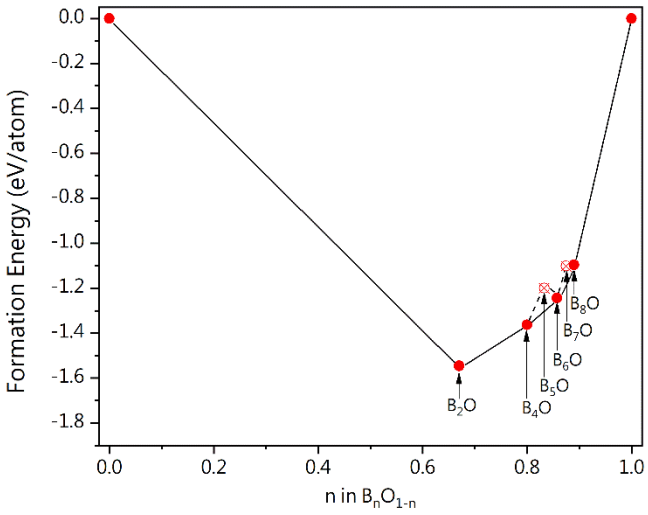

Figure S4. The convex hull of 2D planar boron oxides. the boron oxides with B/O ratio ranging from 8:1 to 4:1 were taken from the work by Zhang et.al[2], We see that our h-B_2O is indeed located on the convex hull. Therefore, it should be stable.

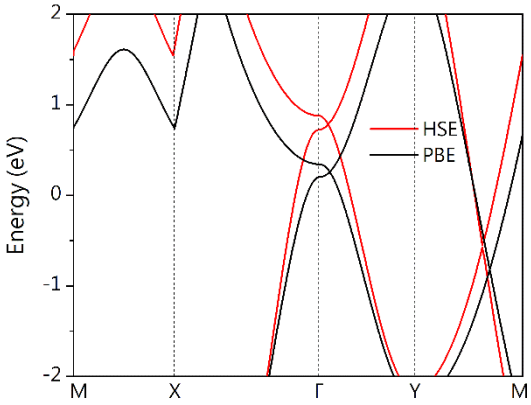

Figure S5. The band structures of h-B_2O at PBE and HSE level. The comparison between HSE and PBE results didn' t show any qualitative change, just the energy window of nodal-loop has been shifted slightly.

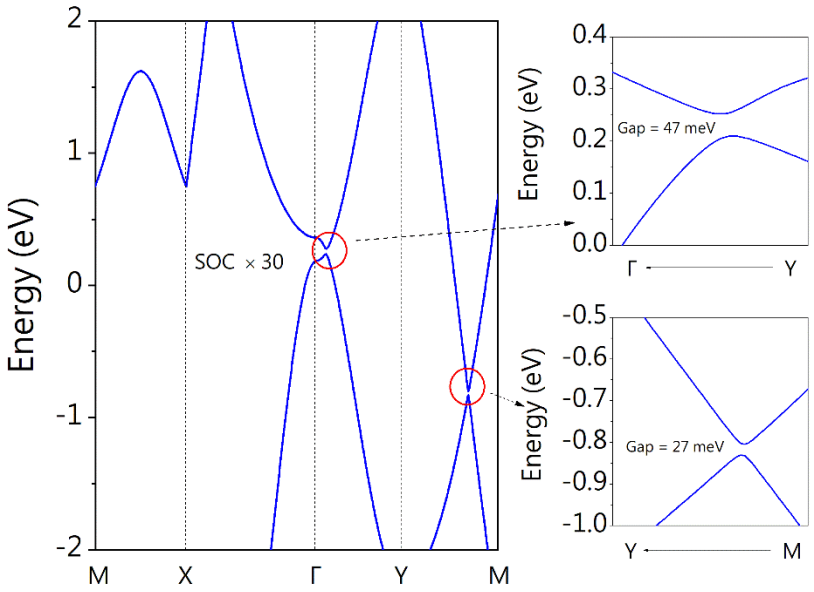

Figure S6. The band structure of h-B_2O with SOC, which is artificially enhanced by 30 times. As shown, the band gap induced by intrinsic strength of SOC of h-B_2O should be the magnitude of 1 meV.

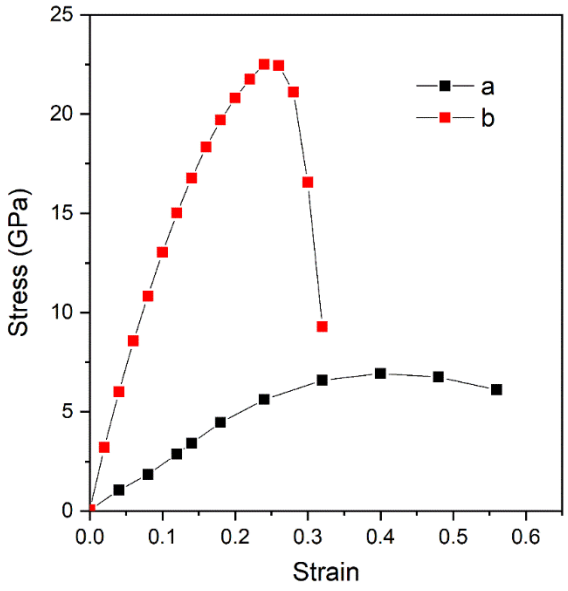

Figure S7. The stress-strain curves of h-B_2O along two lattice directions.

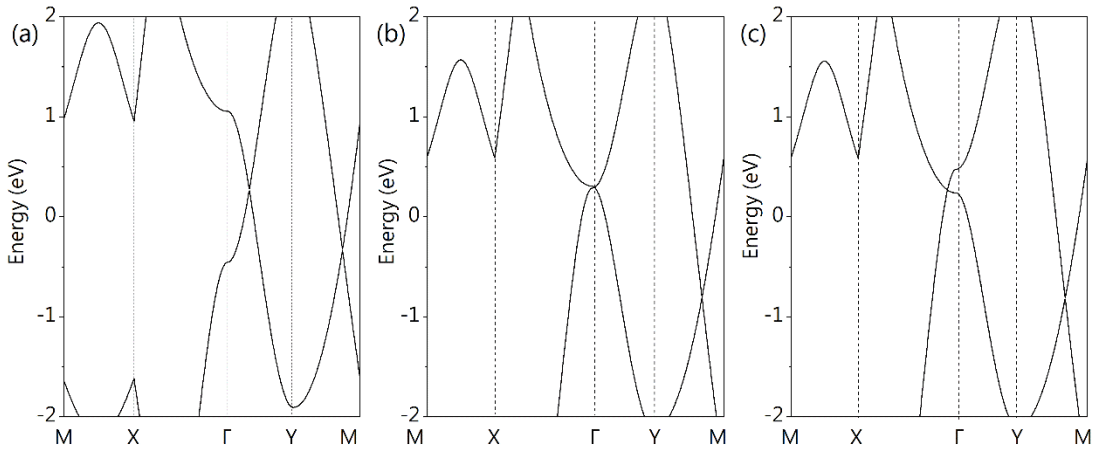

Figure S8. The band structures of h-B_2O under strain of (a) compressive 5%, (b) tensile strain 5.15% and (c) tensile strain 7% along b-axis. Within proper strain along b-axis, the same nodal-loop transformation is still revealed.

Supporting note: The h-B_2O on substrate

Let's talk about the possibility of synthesizing in experiments for h-B_2O. The free-standing hexagonal borophene have been claimed unstable[3], we also calculated its phonon spectra to confirm the instability of free-standing hexagonal borophene, as there are plenty imaginary modes appeared throughout the entire BZ (see Fig S9) . However, with appropriate substrate, the unstable free-standing h-borophene monolayer can be growth successfully on the Al (111) surface[4]. As we mentioned above, the h-B_2O can be viewed as the oxide of hexagonal borophene (see Fig S1), therefore, here we tested the structural integrity of h-B_2O on Al (111) substrate. As we can see from Figure S10, the h-B_2O can maintain its structure quite well.

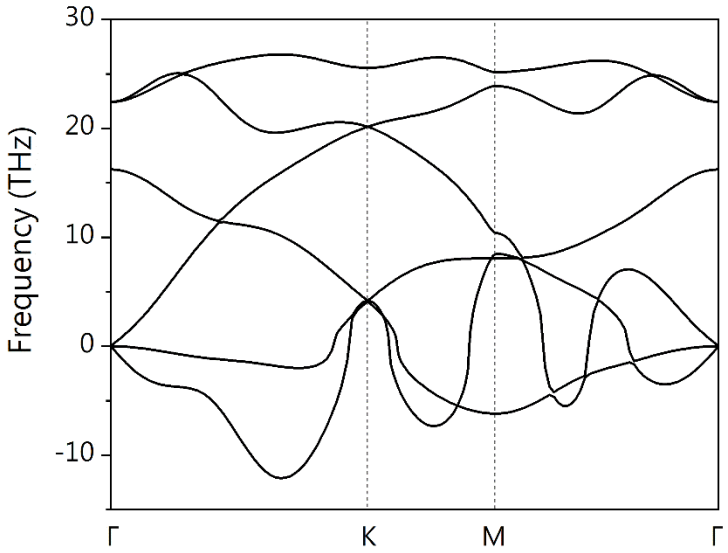

Figure S9. The phonon spectra of free-standing hexagonal borophene.

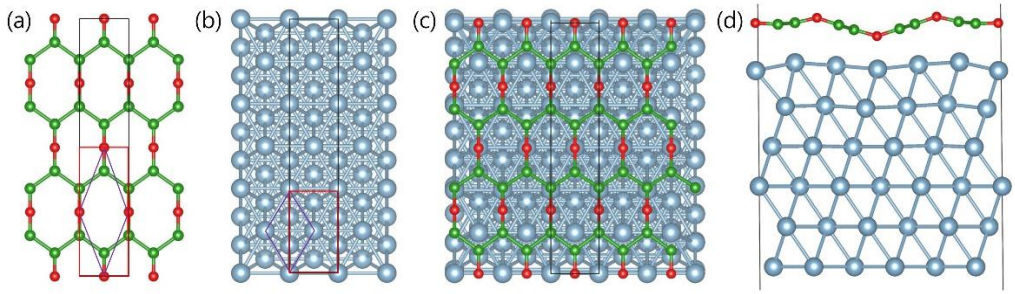

Figure S10. The black lines in (a) and (b) are the co-periodic supercells of 1×2 conventional cell (red lines in (a)) of h-B_2O and 1×3 reshaped unit cell (red lines in (b)). The purple rhombuses in (a) and (b) represent the primitive cell of h-B_2O and Al (111), respectively. With this configuration, the strain of h-B_2O along **a** and **b** directions are 3.66 % and 0.68 %, respectively. (c) and (d) are the top view and side view of h-B_2O on Al (111) substrate after totally structural optimization, showing that the skeleton of h-B_2O is well persevered.

Generally speaking, the electronic band structure of h-B_2O can be affected by the substrate. Here, we have calculated the band structure of h-B_2O on Al (111) substrate, as shown in Figure S11 (a). However, because Al is a metal, the bands of h-B_2O cannot be clearly discerned from the bands of Al substrate. Therefore, in order to probe and utilize the electronic properties, the h-B_2O monolayer should be transferred to some inert substrates, such as BN. Hence, we consider the structure with h-B_2O encapsulated by two BN monolayers, as shown in Figure S11(b). Figure S11(c) shows the corresponding band structure, we see that the linear band dispersions of nodal-loop semimetal around fermi level are indeed well kept.

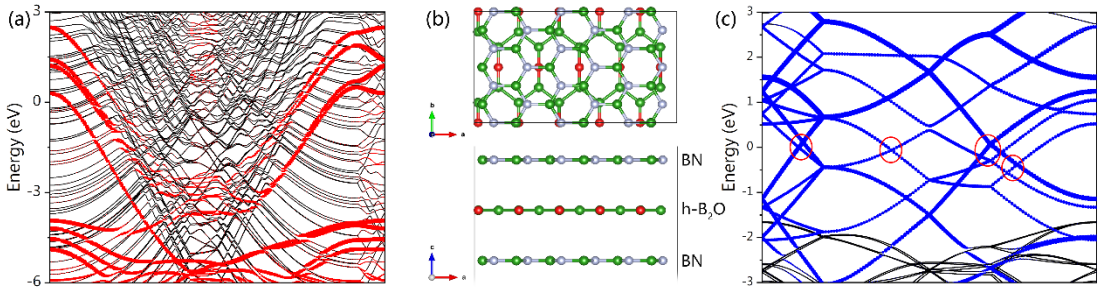

Figure S11. (a) The band structure of h-B_2O on Al (111), the red bands indicate the contribution of h-

B_2O. (b) The top view (up panel) and side view (down panel) of atomic configuration of h-B_2O sandwiched between 2D BN. (c) The band structure of configuration of (b), the blue band indicate the contribution of h-B_2O. The supercell of configuration of (b) leads the Brillouin Zone reduced and the band structures will fold from that of its primitive cell. However, the features of nodal-loop semimetal with linear dispersion bands are still manifested, as marked with red circles.

Supporting references:

1. J. Lu, J. Wu, A. Carvalho, A. Ziletti, H. Liu, J. Tan, Y. Chen, A. H. Castro Neto, B. Özyilmaz and C. H. Sow, *ACS Nano*, 2015, **9**, 10411-10421.
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4. W. Li, L. Kong, C. Chen, J. Gou, S. Sheng, W. Zhang, H. Li, L. Chen, P. Cheng and K. Wu, *Sci. Bull.*, 2018, **63**, 282-286.