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

Supplementary Information for

Two-dimensional tunable double Weyl fermion in BL-α borophene

Xiaoyu Wei,[1,2] Lei Jin,[1,2] Xiaoming Zhang,[1,2] Ying Liu,[2] Xuefang Dai,[2*] and Guodong Liu[1,2*]

[1]State Key Laboratory of Reliability and Intelligence of Electrical Equipment, Hebei University of Technology, Tianjin 300130, China.

[2]School of Materials Science and Engineering, Hebei University of Technology, Tianjin 300130, China.

E-mail: xuefangdai@126.com; gdliu1978@126.com

I. Phonon spectrum for BL-α borophene

The dynamic stability of BL-α borophene can be inferred from the phonon spectrum. We calculated the phonon spectrum of 3*3*1 supercell of BL-α borophene. As shown in Fig. S1, one observes that there is no imaginary frequency throughout the whole Brillouin zone, indicating that BL-α borophene is dynamical stable.

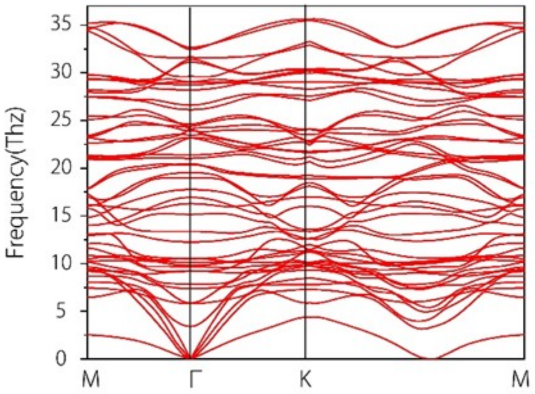

Fig.S1 Phonon spectrum for BL-α borophene.

II. Interlayer interaction of BL-α borophene

We calculated the interlayer interaction by adjusting the interlayer distance d, finding that the BL-α borophene has a strong interlayer interaction. We denote Δd to measure the change in distance between two layers. As shown in Fig.S2 (a), when changing Δd from 0 to 1 Å, the energy undergoes a sharp change, from -93.5 eV to -91 eV, then showing a stable energy. Therefore, the BL shows a strong interlayer interaction, about 322.7 meV/atom[1]. We also find that this strong interlayer interaction comes from the contribution of interlayer covalent bond and van der Waals force. We plot the local charge density to demonstrate this result. As shown in Fig.S2 (b), when Δd is less than 1 Å, it shows a high local charge density between B_1 atoms of two layers, indicating a strong covalent bond. On the contrast, the covalent bond is destroyed when Δd is beyond 1 Å, only the van der Waals force works. To be noted, when $\Delta d \sim 5$ Å, the interlayer van der Waals force is very small, so the interlayer interaction can be ignored. Our discussion about the results of applying strain in the main text is within $\Delta d \in (0,1)$ Å.

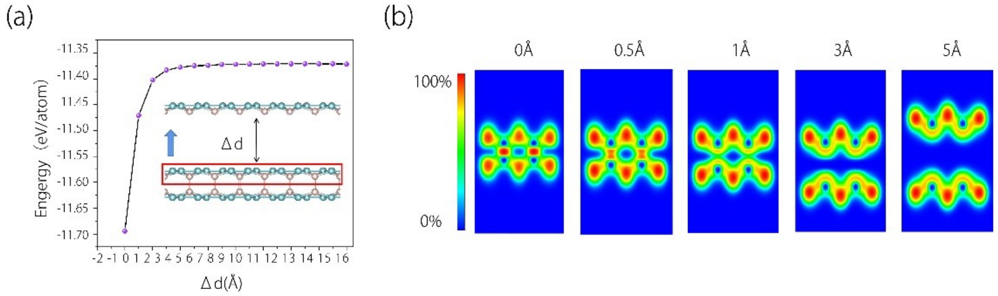

Fig.S2 (a) Curve of interlayer interaction as a function of Δd. (b) 2D slice of local charge density of (-110) plane at different interlayer distances.

II. Buckled structure of BL-α borophene

When applying strain, we also provide the corresponding variation in the crystal structure of BL-α borophene. As shown in Fig.S3 (b), it clearly shows that the layers become much more buckled compared with its original structure, with increasing angle (θ) between two B_2 atoms and the height (h) between B_1 and B_2 in the same layer. At the same time, the bond length of B_1-B_2 becomes shorter. Since the topological properties is strongly related to the structure of materials, as the referee said, it is the buckling along with strain causing interesting topological effects.

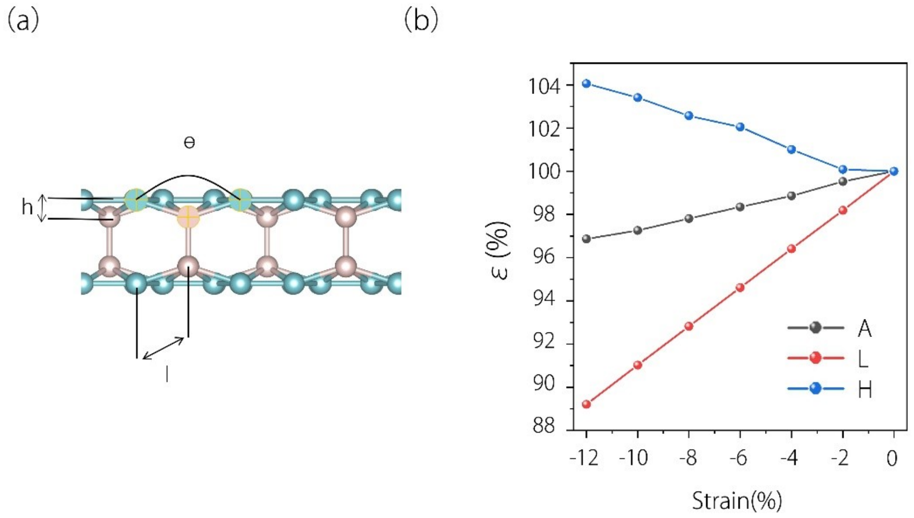

Fig.S3 (a) Side views of BL-α borophene. θ, l and h are respectively B_2-B_1-B_2 bond angle, B_1-B_2 bond length and buckling height. (b) Change trend of L, H and A with strain. θ_0 and l_0, h_0 are the bond angle, bond length and buckling height under no strain, respectively. $A= \theta/ \theta_0$, $L=l/l_0$, $H=h/h_0$.

References

[1] I.V. Lebedeva, A. A. Knizhnik, A.M. Popov, Y. E. Lozovik, B.V. Potapkin, *Phys. Chem. Chem. Phys*. 2011, ***13***, 5687.