A new type of stable borophene with flat-band-induced magnetism

Zhijian Li[1], Yang Xue[3,1], Qingzhao Yao[1], Bao Zhao[3,1], Wei Xu[1], and Zhongqin Yang[1,2]*

1 State Key Laboratory of Surface Physics and Key Laboratory of Computational Physical Sciences (MOE) & Department of Physics, Fudan University, Shanghai 200433, China
2 Shanghai Qi Zhi Institute, Shanghai 200030, China
3 School of Science, East China University of Science and Technology, Shanghai 200237, China
4 School of Physics Science and Information Technology, Shandong Key Laboratory of Optical Communication Science and Technology, Liaocheng University, Liaocheng 252059, China

Abstract

Based on first-principles calculations, we propose a new type of thermally and dynamically stable magnetic borophene (B_{11}) with a tetragonal lattice. The magnetism is found coming from spin polarization of one bonding flat band located at the Fermi level. The strong interactions between the p_z orbitals of the B atoms in the structural unit lead to the formation of the flat bands. One tight binding model is built to comprehend the magnetic mechanism. Biaxial tensile strain (2.0%) can trigger a phase transition from a semimetal to a semiconductor in the B_{11} monolayer. Our work provides a new route for designing and achieving two-dimensional magnetic materials with light elements.

Geometry structure and its stability

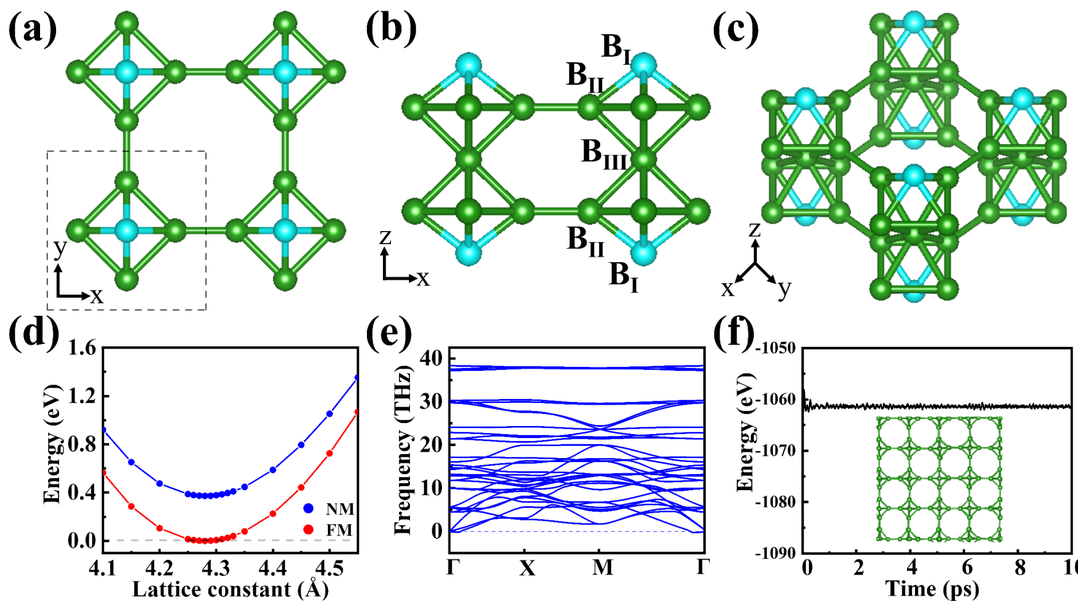

FIG. 1: (a) Top view of the B_{11}. The unit cell is shown with a dashed square. The blue atoms are the magnetic capping atoms. (b) Side view of the B_{11}. The B_I, B_{II}, and B_{III} are the three non-equivalent B atoms. (c) Angle view of the B_{11}. (d) Total energies as a function of the lattice constant for the FM and NM B_{11}, in which the minimum total energy for the FM state is set as energy zero. (e) Calculated phonon spectrum for the FM B_{11}. (f) Calculated energy evolution for the FM B_{11} at 133 K. The inset gives the snapshot of the final frame in the MD simulation.

TB model

One TB model is constructed to understand and generalize the magnetism.

$$H(k) = H_{on\ site}(k) + H_{hop}(k)$$

where $H_{on\ site}(k)$ and $H_{hop}(k)$ express the on site and hopping interactions, respectively. And they are written as

$$H_{on\ site}(k) = \begin{bmatrix} \varepsilon_0 & 0 \\ 0 & \varepsilon_0 \end{bmatrix}$$

$$H_{hop}(k) = \begin{bmatrix} T & t_0 \\ t_0 & T \end{bmatrix}$$

$$T = 2t_1(cosk_x a + cosk_y a)$$

where ε_0 represents the on-site energy of the top/bottom site, t_0 represents the strength of hopping interactions between the top and bottom sites mediated by the effective bridging atom in the structural unit, and t_1 represents the strength of hopping interactions between the sites in the nearest-neighboring unit cells. We can solve the equation to get the $E(k)$,

$$E(k) = \varepsilon_0 \pm t_0 + 2T$$

Magnetism mechanism

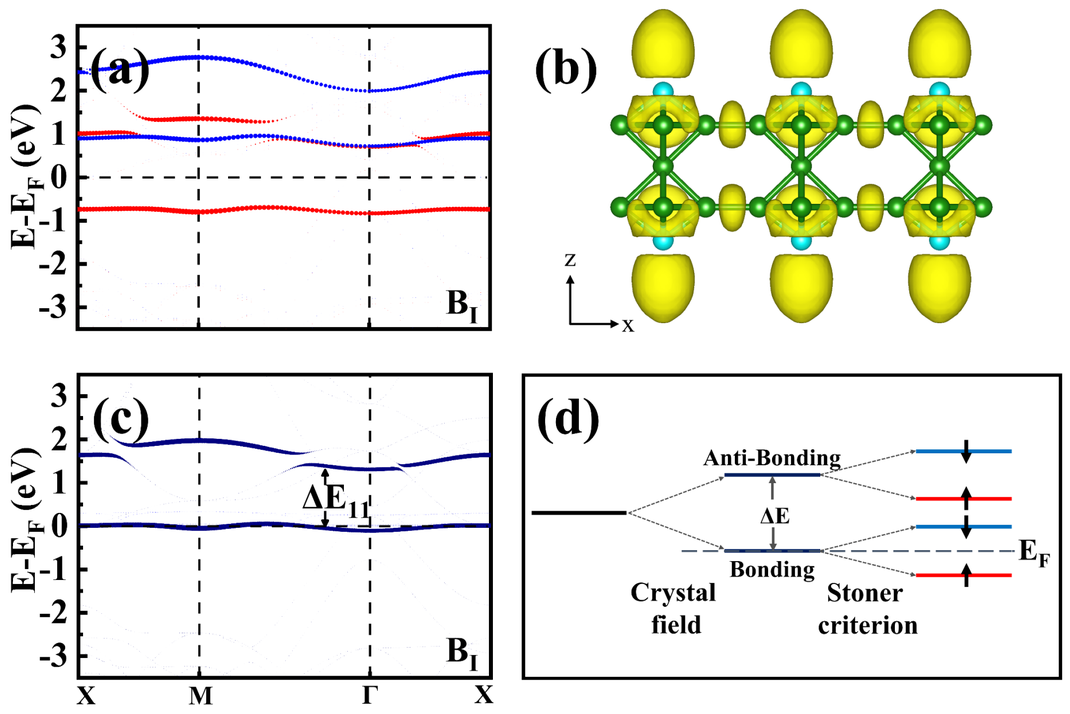

FIG. 3: (a) Projected bands of the B_I p_z orbital in the FM B_{11}. (b) Side view of the ELF of the FM borophene. (c) Projected bands of the $B_I p_z$ orbital in the NM B_{11}. ΔE_{11} expresses the splitting strength of the $B_I p_z$ bonding and anti-bonding states. (d) Magnetism mechanism diagram of the B_{11}.

Electronic Structures

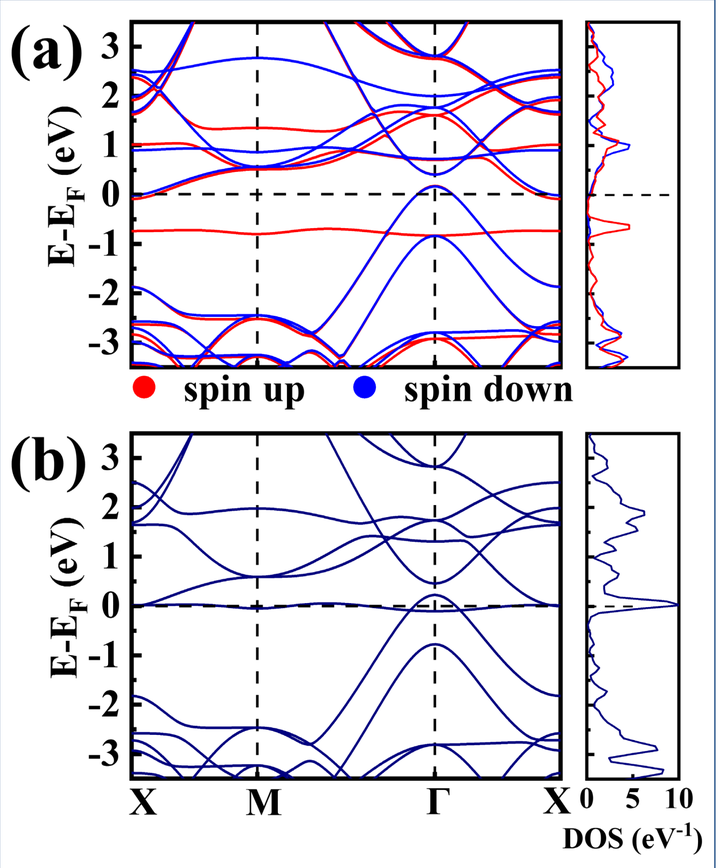

FIG. 2: (a) Band structures and DOSs for the magnetic B_{11}. The red and blue curves give the spin-up and spin-down components, respectively. (b) Band structure and DOS for the NM B_{11}.

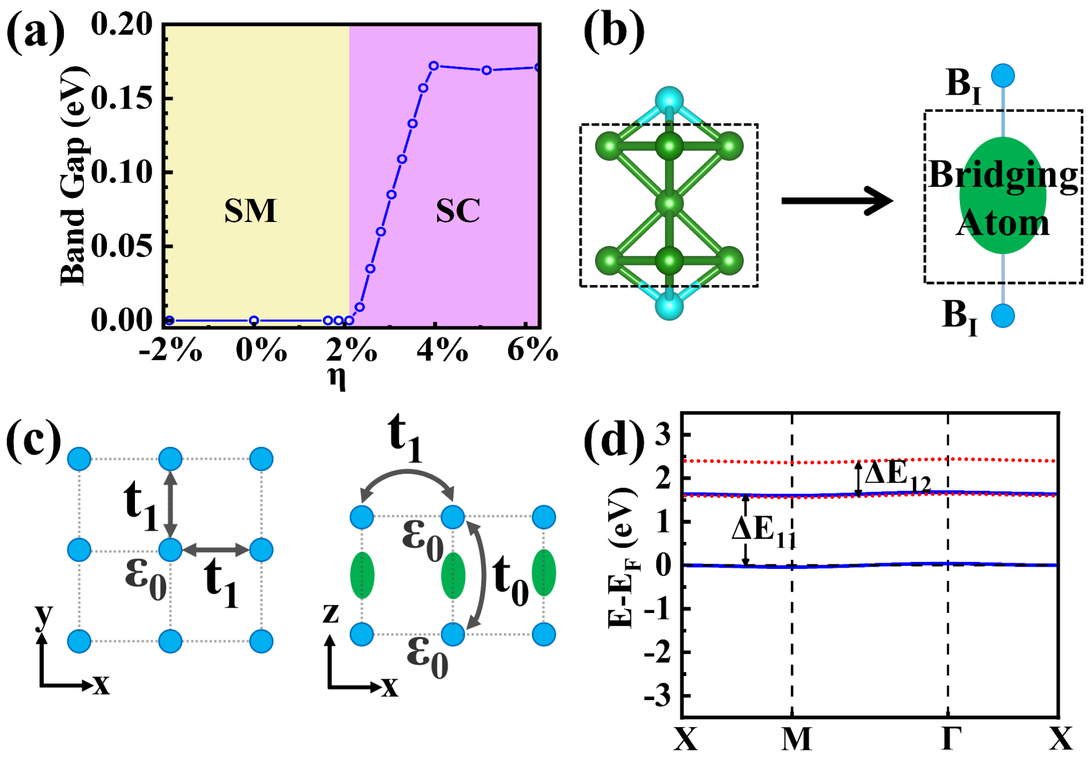

FIG. 4: (a) Band gap for the B_{11} under biaxial strain. The "SM" and "SC" represent the semimetal and semiconductor, respectively. (b) A general model proposed for the magnetism origin. (c) The simplified lattice adoped in the TB model. (d) The obtained TB bands for the B_{11} (blue curves) and B_{12} (red curves), respectively. The parameters for B_{11} are ε_0 =0.8 eV, t_0=0.8 eV, and t_1=0.01 eV. The parameters for B_{12} are ε_0 =2.0 eV, t_0=0.4 eV, and t_1=0.01 eV.

Conclusions

In summary, we have proposed a stable magnetic B_{11} monolayer, which has a tetragonal lattice and is a semimetal. The magnetism is triggered by the bonding flat band, formed due to the strong interactions between the p_z orbitals of the two capping B atoms mediated with middle B atoms in the structural unit. Under biaxial tensile strain, the B_{11} monolayer can transform from a semimetal to a semiconductor with a global band gap up to 171 meV. One tight binding model is constructed to explore and generalize the magnetism. One new borophen of nonmagnetic B_{12} is tuned to being magnetic based on the proposed tight binding model. Our findings expand the 2D magnetic materials and pave a new path for fabricating new 2D magnetic material composed of light elements.

Contact

Zhijian Li
Zhongqin Yang's Group
Email:20210190011@fudan.edu.cn
Phone:18800206382

References

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[2]B. J. Feng, J. Zhang, Q. Zhong, W. B. Li, S. Li, H. Li, P. Cheng, S. Meng, L. Chen, and K. H. Wu, Nat. Chem. **8** (6), 564 (2016).