Prediction of 2D nodal line semimetals on AA' bilayer black phosphorus

Xiaojuan Liu, Hairui Bao, Guanyi Gao, Yue Li and Zhongqin Yang*

State Key Laboratory of Surface Physics, Key Laboratory for Computational Physical Sciences (MOE) and Department of Physics, Fudan University, Shanghai 200433, China

Introduction

Topological semimetals are a new kind of topological electronic states which are different from topological insulators, Dirac points can form zero-dimension, one-dimension and two-dimension manifolds, as predicted for Dirac/Weyl, nodal line semimetals and topological nodal surface. In the present work, based on density function theory (DFT) and first principles calculations, we propose that AA' bilayer black phosphorus can host a two-dimension topological nodal line semimetal under biaxial compression strain in the absence of spin-orbit coupling (SOC). A close nodal line degenerate band cross on the fermi level and protected by mirror symmetry, degenerate bands have opposite mirror eigenvalues ± 1 when SOC is ignored. In addition, Multilayers AA' stack BP have the similar results and need smaller biaxial compression strain.

Results

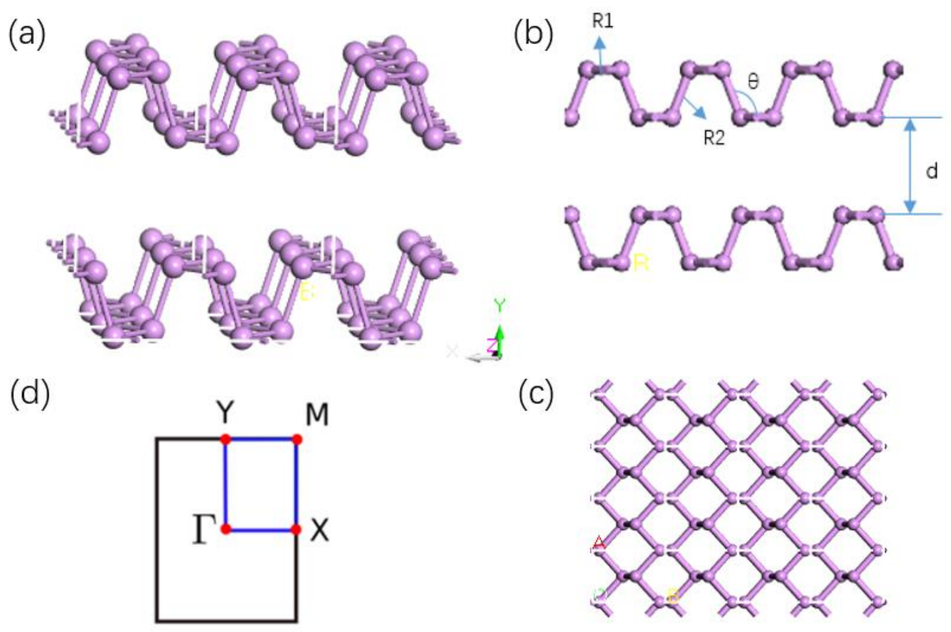

FIG. 1. Geometry structures of AA' bilayer black phosphorus. (a) AA' bilayer black phosphorus crystal structure; (b) side view; (c) top view. (d) 2D first Brillouin zone (BZ)

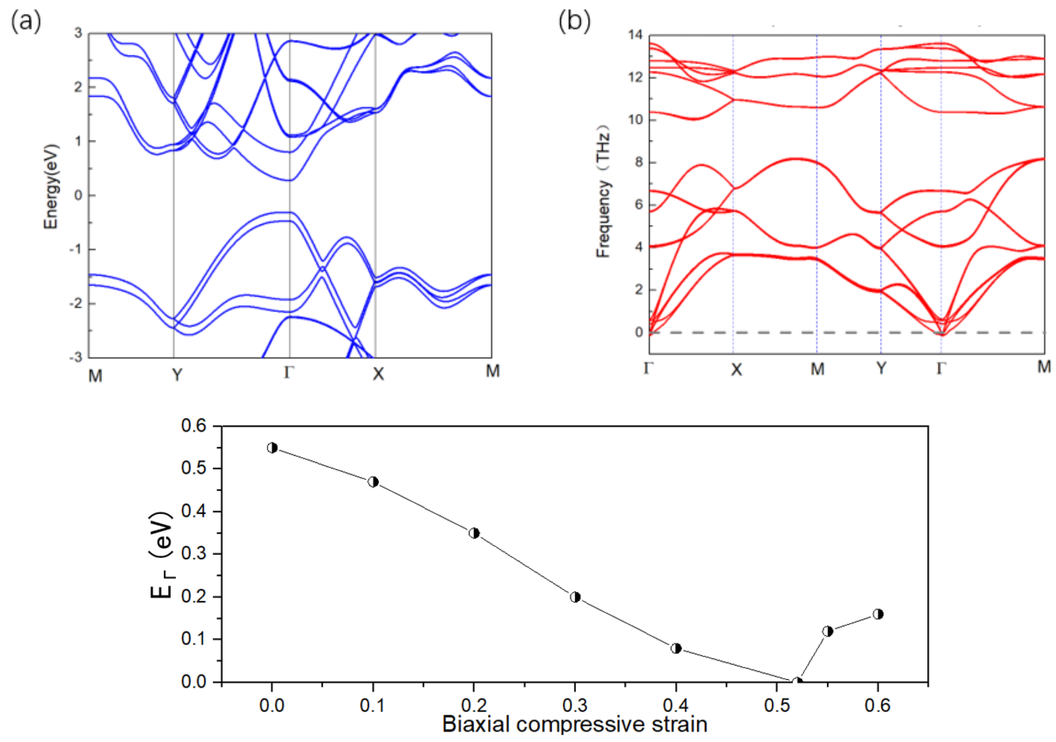

FIG. 2. (a) Band structure of intrinsic AA' bilayer black phosphorus. (b) Phonon spectrum. (c) Energy gap at the Γ point as a function of biaxial compression strain.

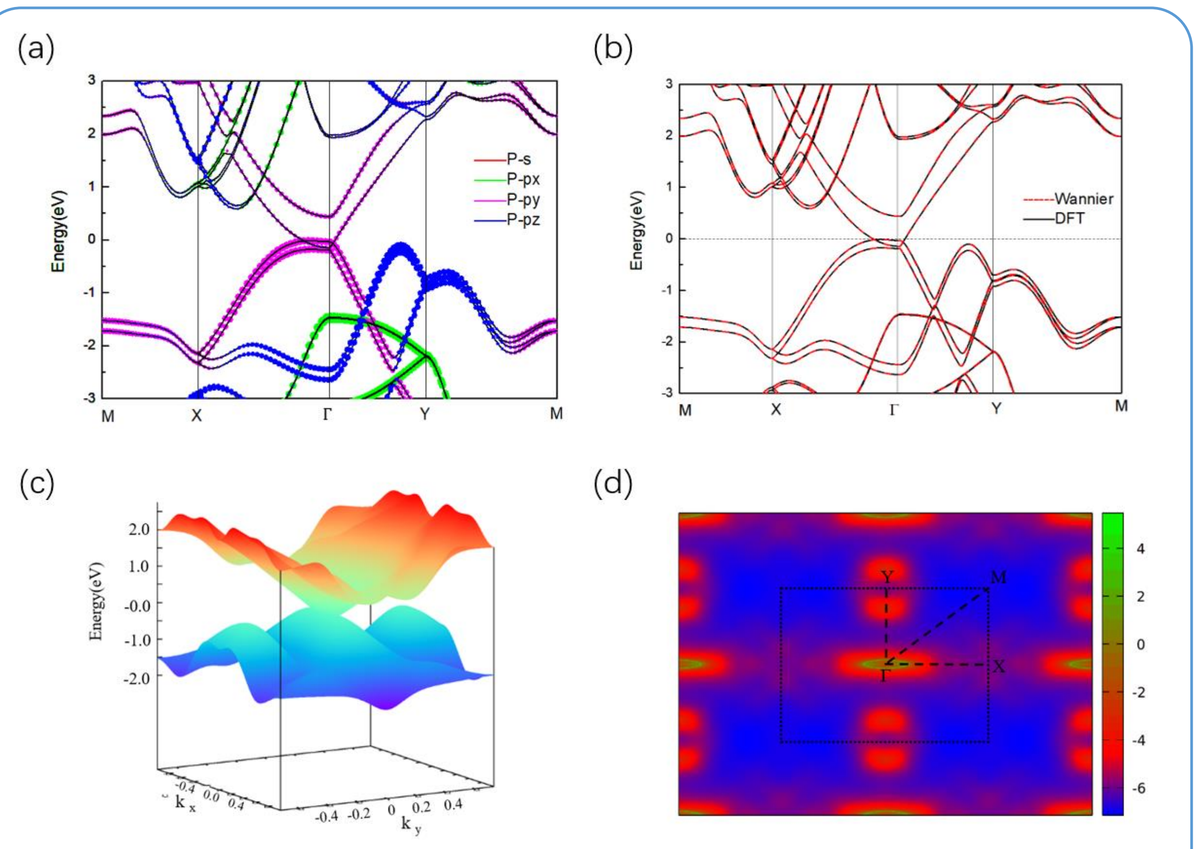

FIG. 3. (a) Orbitally resolved band structure for 5.5% biaxial compression strain of AA' bilayer black phosphorus (without SOC). (b) Band structures for the AA' bilayer black phosphorus without SOC by using DFT methods (black solid line) and Wannier interpretation (red imaginary line). (c) 3D band structure. (d) Fermi surface.

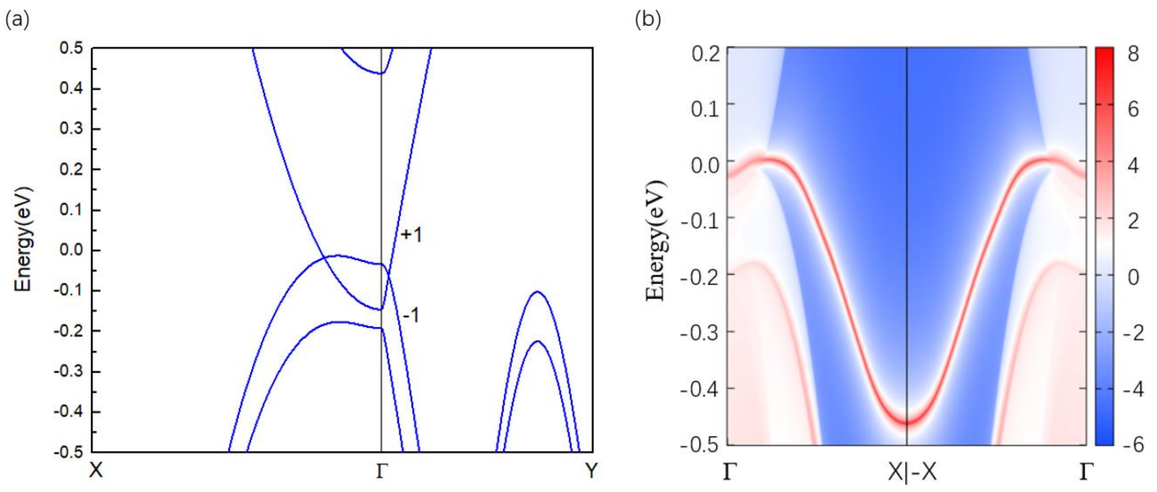

FIG. 4. (a) Band crossing of the bands near the Fermi level form a nodal line, which is protected by the mirror symmetry $x \rightarrow -x$, the bands can be assigned a mirror eigenvalue ± 1 around the Γ point. (b) The edge state of semi-infinite zigzag ribbon of AA'bilayer black phosphorus.

Conclusions

- AA' bilayer BP form a node-ring near the Fermi level by the biaxial compression strain.
- Nontrivial edge state and opposite mirror eigenvalues predict that AA' bilayer BP is a topological nodal line semimetal.
- Multilayers AA' stack BP have the similar results and need smaller biaxial compression strain.

References

1. **Zhao J , Yu R , Weng H , et al. *Phys. Rev. B* 94, 195104 (2016).**
2. **Dai, J. et al. *J. Phys. Chem. Lett.* 5, 1289-1293 (2014).**
3. **Wang, X. et al. *Nature Nanotech.* 10, 517-521 (2015).**