Liang-Jian Zou*
Zhongyi Wang
Institute of Solid State Physics, Chinese Academy of Sciences, Hefei, 230031, China

zou@theory.issp.ac.cn

Strong Magnetic Field Driven Chiral Density Waves in Pressured Black Phosphorus

It is amazing topic that what the Dirac particles behave when Dirac semimetal is under strong magnetic field and in the quantum limit. A few recent work suggested that under strong magnetic field the Dirac or Weyl fermions may become of charge density wave order [1] or helical spin density wave order [2]. In this wok, we demonstrate that the hydrostatically pressured black phosphorus could be tuned from semiconductive to 3D Dirac semimetallic, and under strong magnetic it may evolve into chiral density wave order in the quantum limit. By implementing several codes for searching crystal structures under hydrostatic pressures and first-principles electronic structure calculation together with detailed analytical study, we show that the energy bands crossover around the critical pressure Pc=1.23 GPa. With the increase of magnetic field to strong quantum limit, the Dirac particles in pressured black phosphorus, which is a 3D Dirac semimetal, may become instable and transit to one-dimensional density wave ordering, since the tunning of magnetic field drives the occurrence of Fermi surface nesting. We argue that such a density wave is chiral and is protected by the nonsymmorphic space symmetry of bulk black phosphorus.

References

1. Kai-Yu Yang, Yuan-Ming Lu, and Ying Ran, Phys. Rev. B 84, 075129 (2011)
2. Xiao-Qi Sun, Shou-Cheng Zhang, and Zhong Wang, Phys. Rev. Lett. 115, 076802 (2015)