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First-principles study of band-gap inverted bulk black phosphorus HAN-GYU KIM, HYOUNG JOON CHOI, Department of Physics, IPAP, and Center for Computational Studies of Advanced Electronic Material Properties, Yonsei University, Seoul 03722, Korea — We performed first-principles calculations to study effects of spin-orbit coupling on the electronic band structure of bulk black phosphorus (BP) when the conduction band minimum and the valence band maximum are inverted. Without the spin-orbit coupling, our calculation shows that the crossing points of the valence and conduction bands in the band-gap inverted bulk BP form a closed loop in the momentum space. When we include the spin-orbit coupling in our calculations, the crossing of the valence and conduction bands is lifted at every point in the loop with k-dependent splitting size. We discuss the effects of spin-orbit coupling in band-gap inverted bulk BP by analyzing the symmetry of the atomic structure and the orbital character of the wave functions. This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2016-C3-0052).

Han-gyu Kim
Yonsei Univ

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