Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Quasi-particle band structure of potassium-doped few-layer black phosphorus with GW approximation HAN-GYU KIM, SEUNG SU BAIK, HYOUNG JOON CHOI, Department of Physics, IPAP, and Center for Computational Studies of Advanced Electronic Material Properties, Yonsei University, Seoul, Korea — We calculate the quasi-particle band structure of pristine and potassium-doped black phosphorus (BP) by using the GW approximation. We obtain band gaps of pristine bulk and few-layer BP and compare them with the result of the density functional calculations and experimental measurements. For potassium-doped cases, we calculate the electronic band structure of potassium-doped few-layer BPs with various doping densities. We obtain the critical doping density for the band-gap closing, and the energy-band dispersions when the band gap is inverted. We discuss Dirac semimetal properties of doped few-layer BPs obtained by the GW approximation. This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2015-C3-039).

Department of Physics, IPAP, and Center for Computational Studies of Advanced Electronic Material Properti

Date submitted: 06 Nov 2015 Electronic form version 1.4