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Tunability of Band Gap in Multilayer Phosphorene by External Electric Fields and Electron Dopings SEUNG SU BAIK, HYOUNG JOON CHOI, Center for Computational Studies of Advanced Electronic Material Properties (CCSAEMP) and Department of Physics, Yonsei University, Korea — Black phosphorus (BP) and its two-dimensional derivative phosphorene are rapidly emerging nanoelectronic materials with potential applicability to field effect transistors and optoelectronic devices. Unlike the gapless semiconductor graphene, multilayer BP has a substantial band gap of ~ 0.2 eV and the band-gap size is reportedly varied by external electric fields. To explore the extensibility of such band-gap modulation, we have investigated electronic band structures of multilayer BP by using the first-principles density-functional method as implemented in the SIESTA code. By controlling the electron doping concentrations and the resultant electric fields therefrom, we examine the manageability of the band-gap size and the anisotropic carrier mobility. This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2013-C3-062).

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