Interlayer Interaction that is Decisive in the Energy Gap of a Few Layer Phosphorene

YUKI SUGIHARA, ATSUSHI OSHIYAMA, Dept. of App. Phys., Univ. of Tokyo — We report on our first-principles calculations that clarify the microscopic origin of the band-gap variation in a few-layer phosphorene (i.e. layered phosphorous) and also rectify a prevailed picture of the electronic structure of this new layered material [1]. Calculations have been done either using GGA with inclusion of van der Waals correction in the density-functional theory or GW approximation in the self-energy. We unequivocally reveal that the interlayer interaction causes the bonding-antibonding splitting of the highest valence band state, thus reducing the fundamental energy gap. This is due to the highest state consists mainly of \( p \) orbitals along the direction perpendicular to the layers. It was predicted that phosphorene has four polytypes named \( \alpha \) (black), \( \beta \) (blue), \( \gamma \) and \( \delta \) and all these polytypes exhibit common feature of the band-gap variation [2]. Especially, \( \gamma \) phosphorene is proposed to show the metal-insulator transition from the semiconductor mono-layer to the metal bi-layer. We reveal that this transition takes place in thicker region. [1]L. Li, Y. Yu, G. J. Ye, Q. Ge, X. ou, H. Wu, D. Feng, X. H. Chen, and Y. Zhang, Nat. Nanotechnol. 9, 372 (2014), [2] J. Guan, Z. Zhu, and D. Tomanek, PRL, 113, 046804 (2014)