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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 α (black), β (blue), γ and δ and all these polytypes exhibit common feature of the band-gap variation [2]. Especially, γ 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)

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