Electronic and optical properties of phosphorene/graphene van der Waals heterostructures

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After a series of two-dimensional (2D) layered materials emerging with unique properties [1], van der Waals (vdW) heterostructures have been proposed to design 2D materials with desired properties for various applications [2], such as transistors [3], lasers [4], modulators [5] and detectors [6]. Phosphorene is an increasingly attractive 2D material because of its peculiar properties. Graphene has usually been used to protect phosphorene from degradation for applications [7]. In this work, we systematically investigated the stacking characteristics, electronic structures, band edge alignments and optical properties of all three kinds of stable phosphorene/graphene (P/G) vdW heterostructures in details based on first-principles calculations within the framework of vdW corrected density functional theory [8]. It is interesting that the same stable heterostructures with different lattice mismatch will exhibit different electronic and optical properties. In the heterostructure, the band gap of graphene is almost unchanged when the strain changes from 0 to 3%, while the band gap of phosphorene largely decreases from 1eV to 0.15eV, but always the direct band gap when the strain changes from 0 to 2.8%. In particular, vdW interaction will further increase the gap of phosphorene. We further calculated the optical properties by the photon wavelength dependent dielectric function [9] and find that the strain does not dramatically change the optical properties of graphene but significantly affects that of phosphorene and P/G vdW heterostructures. This work may enhance the understanding of electronic and optical properties of P/G vdW heterostructures and indicate potential reference information for nanoelectronic and optoelectronic applications.

Figure 1. Configuration, band spectrums and corresponding dielectric function (orange line: phosphorene; blue line: graphene; purple line: heterostructure). The percents represent the inhomogeneous strain originating from lattice mismatch.


