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Electric-field tunable electronic properties and Schottky contact of graphene/phosphorene heterostructure

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Abstract

In this paper, we study the electronic properties of graphene/phosphorene (G/P) heterostructure under applied electric field. The interlayer distance between graphene and top-most phosphorene is 3.50 Å and the binding energy per carbon atom is 28.2 meV, which is indicated that graphene is bound to phosphorene via vdW interaction. The appearance of an energy gap of 33 meV in graphene is due to the dominant influence exerted by the phosphorene on graphene and sublattice symmetry broken between graphene and substrate. The G/P heterostructure forms a *p*-type Schottky contact with $\Phi_{Bp} = 0.34$ eV. By applying the negative electric field, the G/P heterostructure keeps a *p*-type Schottky contact. Whereas with the positive electric field of $E \geq +0.25$ V/Å, Φ_{Bp} becomes larger than Φ_{Bn} , resulting in a transformation from *p*-type to *n*-type Schottky contact. The present results may open up a new avenue for application of the G/P vdW heterostructure in electronic devices.

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