Supporting Information

Tuning the Schottky Contacts in Phosphorene and Graphene Heterostructure by the Strains

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S1：The variation tendency of VBM, CBM and band gaps of phoshorene monolayers is similar to the phosphorene in the P-G heterostructures under the strain from -6% to 6%. It illustrates that the P-G vdW heterostructure can preserve the intrinsic electronic excellent properties of the 2D dissimilar materials under different stresses. As the variation of the work function of the phosphorene monolayer and the graphene electrode and the Fermi level shift in the P-G heterostructures, the line of CBM and VBM intersect between the strain of -4% and -2%, showed in Figure 4(a), where the Schottky barrier occurs transition of schottky barrier from n-type Schottky contact to p-type Schottky contact.

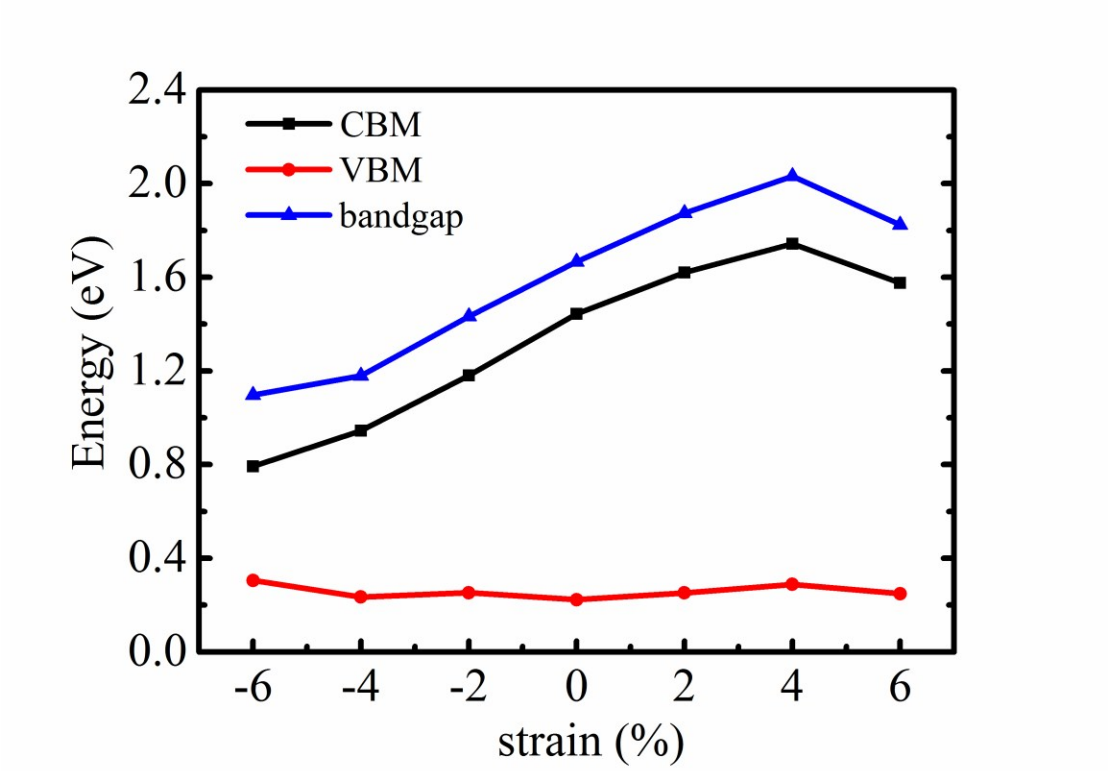

Figure S1: CBM, VBM and bandgap of phosphorene monolayer as a function of the strains.

S2 : Band structures and PDOS of P-p_x, P-p_y and P-p_z orbits of P atoms under the strain of -3.4% in the P-G heterostructure

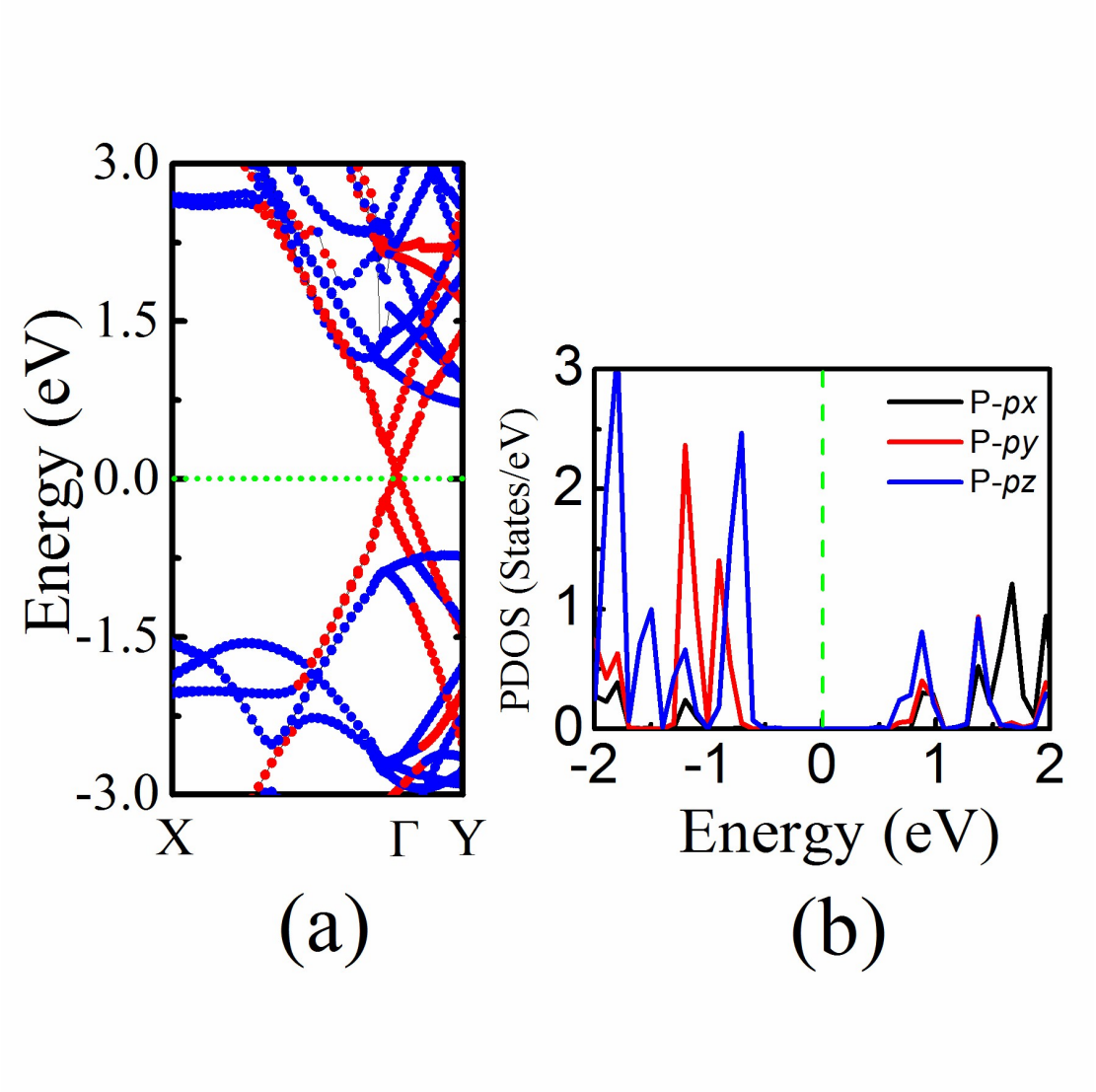

Figure S2: (a) Band structures of the P-G heterostructure under the strain of -3.4%. Blue and red denote the contributions from phosphorene monolayer and graphene, respectively. The FL is set to zero and marked by green dotted line. (b) PDOS of P-p_x, P-p_y and P-p_z orbits of P atoms under the strain of -3.4%. The FL is set to zero and marked by green vertical dotted line.