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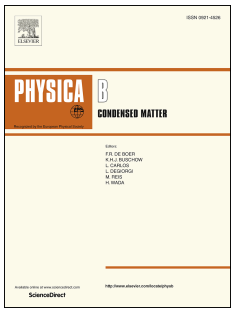

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Interlayer coupling effects on Electronic properties of the phosphorene/h-BN van der Walls heterostructure: a first principles investigation

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ABSTRACT

By using first-principles calculations, we systemically investigate the electronic properties of phosphorene/*h*-BN heterostructure with different interlayer distances. Our results show that the electronic states in the vicinity of the Fermi level are completely dominated by phosphorene, and the system exhibits type-I band alignment consequently. Moreover, we also reveal the variation of the band structure of phosphorene/*h*-BN heterostructure with different interlayer distances. The band gap undergoes a direct to indirect transition as decreasing the interlayer distance. The mechanism of the band gap transition can be attributed to the different energy levels shifts, according to different electronic orbital characters on the band edge. In specific, the energy level of the P_p_z bonding state shifts up while that of the P_p_x,p_y bonding state falls down, along with the enhancement of the