Tunable band alignment in boron carbon nitride and blue phosphorene van der Waals heterostructure

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Abstract

The hybrid monolayer of boron nitride and graphene, namely the BC\(_3\)N monolayer, has been recently revealed as a direct bandgap semiconductor with exceptional thermal, mechanical and optical properties. The integration of such monolayer with other 2D materials into a van der Waals heterostructure (VDWH), however, remains largely unexplored thus far. In this work, we investigate the electronic and structural properties of a new class of VDWH obtained via the vertical stacking of BC\(_3\)N and blue phosphorene monolayers. By using first-principle density functional theory (DFT) simulation, we show that BC\(_3\)N couples to the blue phosphorene layer via weak van der Waals interactions and exhibits a type-II band alignment which is beneficial for electron-hole pair separation in photodetection and solar cell applications. Intriguingly, changing the interlayer separation induces an indirect-to-direct band gap transition which changes the band alignment types of the VDWH. The interlayer separation, which can be readily tuned via a vertical strain, thus provides a useful tuning knob for switching the heterostructures between type-I and type-II VDWHs. Our findings reveals the BC\(_3\)N-based VDWH as a versatile material platform with tunable band alignments, thus opening a route towards novel VDWH-based optoelectronic devices.

1. Introduction

The emerging class of two-dimensional (2D) materials offer an intriguing material platforms that covers an enormously broad spectrum of solid states, including metal, semiconductor, insulator, superconductor, Mott insulator, and so on. By vertically stacking different 2D materials into van der Waals heterostructures (VDWHs) [1–5], the physical properties of the resulting hybrid structures can be artificially integrated and engineered. 2D materials and their nearly unlimited combinations to form VDWHs thus provide a new paradigm shift in material science, condensed matter physics and device engineering [6–10].

One of the crucial control parameters of VDWHs is the band alignment between the 2D layers, which can be classified into three distinct types, namely the (i) type-I straddling gap; (ii) type-II staggered gap; and (iii) type-III broken gap VDWHs [11]. The electronic properties of the VDWHs is sensitively influenced by the band alignment types. For example, the optical devices, such as light-emitting diodes and lasers, are usually prepared using the type-I heterostructures which promotes carrier recombination [12]. On the other hand, type-II heterostructures are most widely useful applications where efficient electron-hole pair separation and weak recombination are preferred, such as photodetection, and also for unipolar electronic device [13]. A versatile strategy of band alignment engineering in VDWHs is thus a key challenge towards the development of broad electronic and optoelectronic applications using 2D materials [14].

Recently, graphene-like materials, such as boron-carbide (BC\(_3\)) and carbon-nitride (C\(_3\)N) which similarly has a honeycomb lattice, have been extensively studied [15–20]. BC\(_3\)N exhibits various electronic properties depending the mixing ratio and arrangement of atoms [21, 22]. For instance, BC\(_3\)N and BC\(_3\)N are
semiconductors with a direct band gap of about 1.57 eV [23] and 1.26 eV [24], respectively. These 2D semiconductors exhibit strong potential in many device applications owing to their outstanding mechanical, optical, electronic and thermal properties [25, 26]. The carrier mobility of few-layer BC2N can reach \(8 \times 10^6\) cm\(^2\) V\(^{-1}\) s\(^{-1}\), which is highly relevant for high-performance nanoelectronic applications [23].

Theoretical studies further predict defective and doped BC2N monolayer exhibit excellent electrochemical properties, thus serving as a good anchoring materials for Li-S batteries [27]. Although multiple theoretical and experimental works have been devoted to unearth the unusual physical properties of BC2N nano- and few-layers, the fusion of BC2N with other 2D monolayers to form VDWHs remain largely unexplored thus far.

In this work, we propose a new class of VDWH composed exclusively of honeycomb-type lattices, namely the vertical stacking of flat honeycomb lattice, BC2N, and buckled honeycomb lattice, blue phosphorene—a 2D monolayer in the phosphorene family that exhibits superb electronic properties and has been successfully synthesized on an Au(111) substrate using molecular beam epitaxy technique [28–31]. Recently, the integration of blue phosphorene with graphene [32, 33], transition metal dichalcogenides [34, 35], and other 2D materials [36] have been extensively explored, which reveals blue phosphorene as a versatile building block for designing VDWHs. Here we study the electronic properties of two species of the boron-carbon–nitride/blue-phosphorene VDWHs, namely the BC2N/Blue phosphorous (BC2N/P) and BC6N/Blue phosphorous (BC6N/P), by performing first principles density functional theory (DFT) calculations. We show that both BC2N and BC6N monolayers couple weakly to the blue phosphorene via van der Waals interactions, thus preserving the pristine electron properties of the 2D monolayers after forming the heterostructures. Furthermore, the two heterostructures exhibit intrinsically type-II energy band alignment at equilibrium. The band gap of the heterostructures can be tuned by varying the vertical interlayer separation between the boron carbide nitride monolayer and the blue phosphorene, which can be achieved via an external vertical strain. Intriguingly, such tunable band gap directly leads to the switching of the heterostructures band alignment between type-I to type-II. Our findings thus suggest that the exclusively honeycomb-lattice-based boron-carbide/blue-phosphorene VDWHs proposed here may serve as a versatile material platform for both the exploration of the fundamental light–matter interaction at reduced dimensionality and the practical design of novel optical and optoelectronic devices.

2. Computational details

First-principles calculations were performed in this work by employing the Vienna ab-initio Simulation Package (VASP) [38, 40]. The plane-wave method within the Perdew–Burke–Ernzerhof (PBE) form of the generalized gradient approximation (GGA) for the exchange correlation potential is implemented [41]. The cutoff energy of 500 eV is used, and 9 \(\times\) 9 \(\times\) 1 \(k\)-points in the Brillouin zone are sampled. To avoid the artificial interactions between adjacent layers, a 20 Å vacuum layer is chosen along the z direction. All the atomic positions are fully relaxed and the convergence criteria are set as 10\(^{-6}\) eV for the total energy and 0.01 eV Å\(^{-1}\) for the forces. We used the DFT-D3 method of Grimme to correctly describe the effect of interlayer vdW interaction [42].

3. Results and discussions

To construct the BC2N/P VDWHs, we first investigated the structural parameters of BC2N, BC6N, and Blue phosphorus. The lattice constants of BC2N, BC6N, and blue phosphorus monolayers are 5.01, 4.979 and 3.279 Å, respectively, which are consistent with that reported in the literature [24, 43, 44]. When constructing the BC2N/P heterostructures, we have considered surface periodicities of \(\sqrt{3}\) \(\times\) \(\sqrt{3}\) for BC2N and BC6N, and \(\sqrt{7}\) \(\times\) \(\sqrt{7}\) for blue phosphorus, so to reduce the lattice mismatch. All the atomic positions and the lattice vectors of BC2N/P and BC6N/P are fully relaxed (see figure 1). The optimized lattice constants are 8.64 Å for BC2N/P, 8.61 Å for BC6N/P, and the corresponding lattice mismatches are all less than 1%. The vertical interlayer distances are 3.408 Å for BC2N/P and 3.466 Å for BC6N/P, which are larger than the sum of the covalent radii of B, C, N, and P atoms. Thus, weak van der Waals interactions are dominant without chemical bonding at the vertical interface region between BC2N and blue phosphorene.

By comparing the total energies of the final heterostructures systems, we examined the stability of BC2N/P and BC6N/P by calculating the binding energy, \(E_b\), defined as

\[
E_b = E_{BC2N/P(BC6N/P)} - E_{BC2N(NC6N)} - E_p,
\]

where \(E_{BC2N/P(BC6N/P)}\) is the energy of the combined systems, \(E_{BC2N(NC6N)}\) and \(E_p\) are the energies of the isolated monolayer BC2N (BC6N) and blue phosphorene, respectively. We found that the values of the \(E_b\) of the relaxed BC2N/P and BC6N/P VDWHs are \(-6.078\) and \(-6.088\) eV, respectively, at the equilibrium. According to the formula, the formation energy is negative which means that the formation of BC2N and Blue phosphorene
heterostructure is an exothermic process, which indicates the thermodynamical stability of the structure. In figures 1 (g) and (h), we present the calculated evolution of the corresponding binding energy with interlayer distance (figure 1(g)) and displacements $\delta_{xy}$ (figure 1(h)) of the BC$_2$N layer relative to blue phosphorene. It can be seen that the evolution behaviors of the $E_b$ are similar with the interlayer distance and interface displacement for the two considered systems.

To understand the electronic structures of BC$_2$N/P and BC$_6$N/P VDWHs, we first calculate the electronic band structures of the free standing isolated BC$_2$N (figure 2(a)), BC$_6$N (figure 2(b)) and blue phosphorene monolayer (figure 2(c)) in terms of the unit cell (black short dot) and the super cell (blue or red solid line). BC$_2$N and BC$_6$N monolayers are direct gap semiconductor with the conduction band minimum (CBM) and the valence band maximum (VBM) located at $\Gamma$ point. The CBM and VBM of BC$_2$N are mapped to the $\Gamma$ point in the supercell as similar to graphene [45, 46]. The band gap are 1.594 eV for BC$_2$N, and 1.276 eV for BC$_6$N, which agree well with previous works [23, 24]. In contrast, blue phosphorene is an indirect semiconductor, and the calculated indirect band gap value is 1.927 eV. Next, we present the projected band structures of the BC$_2$N/P and BC$_6$N/P VDWHs in figures 2(d) and (e), respectively. Compared with those of the isolated monolayer BC$_2$N, BC$_6$N and Blue phosphorene, the electronic structures of BC$_2$N, BC$_6$N and Blue phosphorene are well preserved upon forming the heterostructures. Both BC$_2$N/P and BC$_6$N/P heterostructures display a semiconducting characteristics with an indirect band gap of 1.112 eV and 1.103 eV, respectively. The CBM of BC$_2$N/P and BC$_6$N/P heterostructures are localized at Blue phosphorene component. In contrast, the VBM of these heterostructures are mainly contributed by the electronic states in BC$_2$N and BC$_6$N layers. Thus, type-II band alignment is formed in the BC$_2$N/P and BC$_6$N/P heterostructures. Because type-II band alignment can effectively facilitate the separation of electron-hole pair, the BC$_2$N/P heterostructures are expected to hold potential in optoelectronic applications where electron-hole separations are preferred, such as photodetector and solar cell.
We further calculate the work functions and the band alignment of BC\textsubscript{x}N/P heterostructure relative to the vacuum level in figure 4. The work function is the energy difference between the Fermi level E\textsubscript{F} and the vacuum level E\textsubscript{vacuum}. As depicted in figure 3(a), the work functions of monolayer BC\textsubscript{2}N, BC\textsubscript{6}N, P, BC\textsubscript{2}N/P, and BC\textsubscript{6}N/P heterostructure are 4.457, 4.299, 5.22, 4.772, and 4.743 eV, respectively. The work functions of both heterostructures lies between the BC\textsubscript{x}N (higher work function) and blue phosphorene (lower work function).

When the BC\textsubscript{x}N monolayer comes in contact with blue phosphorene, there is an electron flow from BC\textsubscript{x}N monolayer to the blue phosphorene because of the lower work function of blue phosphorene. The Fermi level of BC\textsubscript{x}N monolayer shift downwards while the Fermi level of Blue phosphorene shifts upwards, thus leading to the formation of an intrinsic type-II band alignment as illustrated in figures 3(b) and 3(c). The conduction band offset $\Delta E_{c}$ of BC\textsubscript{2}N/P and BC\textsubscript{6}N/P are calculated to be 0.455 eV and 0.148 eV, respectively, while valence band offset $\Delta E_{v}$ of BC\textsubscript{2}N/P and BC\textsubscript{6}N/P are calculated to be 0.776 eV and 0.661 eV, respectively. The conduction band offsets of BC\textsubscript{2}N/P is thus much larger than that of BC\textsubscript{6}N/P, while the valence band offsets of the two heterostructures are similar.

The significantly shifted band structures after the formation of heterostructure are caused by the charge redistribution at the interface. We calculate the plane-averaged differential charge densities $\Delta \rho$ along the Z-direction of the BC\textsubscript{2}N/P and BC\textsubscript{6}N/P heterostructures, which is defined as

$$\Delta \rho = \rho_{H} - \rho_{BC\textsubscript{x}N} - \rho_{P}$$

where $\rho_{H}$, $\rho_{BC\textsubscript{x}N}$, and $\rho_{P}$ are the charge densities normal to the plane of the BC\textsubscript{x}N/P heterostructures, the BC\textsubscript{x}N and the blue phosphorene, respectively. The calculated $\Delta \rho$ profiles are shown in figures 3(d) and (e). The blue regions and red region represent electron depletion and accumulation of in the heterostructures relative to the two isolated monolayers, respectively. Because the potential and work function of the two materials are different, charge redistribution takes place in the system to form charge depletion (blue isosurface) and accumulation (red isosurface) as depicted in figures 3(d) and (e). In reaching equilibrium, the electrons move from the BC\textsubscript{x}N monolayer to the blue phosphorene monolayer in the interfacial region, which is consistent with the band alignment analysis discussed in figures 3(a)–(c). The transfer of electrons from BC\textsubscript{x}N monolayer continue to the blue phosphorene monolayer causes the electrons to accumulate near the blue phosphorene layer, while the BC\textsubscript{x}N monolayer becomes electron-depleted. This charge redistribution phenomena leads to a built-in electric field directed from BC\textsubscript{x}N monolayer to blue phosphorene monolayer, which further aggravates the drift of holes and electrons, and eventually reaches an equilibrium. An interface dipole is thus formed across the vertical interface [47, 48].
Finally, we investigate the evolution of the band alignment when the interlayer distance between BC\(_x\)N and blue phosphorene is varied, as shown in figure 4. The interlayer spacing has a strong influence on the electronic structure of the heterostructure. When the interlayer distance is close to the covalent radius, the interface coupling intensifies, resulting in the destruction of the electronic structure of BC\(_x\)N, as shown in figures 4(a) and (e). Thus, the band alignment changes from type-I to type-II heterostructures with decreasing interlayer distances for both the BC\(_2\)N/P (figures 4(a) to (c)) and the BC\(_4\)N/P (figures 4(e) to (g)). In figure 4(d) and (h), the band gap evolution of the two heterostructures as a function of the interlayer distance. The maximum band gap signifies the transition from type-II to type-I band alignments. The transition occurs at about 2.9 Å and 3.3 Å for BC\(_2\)N/P and BC\(_4\)N/P, respectively. Below these interlayer distance values, the band alignment evolves into type-I band alignment. Finally, we remark that although the interlayer distance of the VDWHs is not a dynamically adjustable parameter, it can be engineered during the material fabrication processes. Multiple methods can be employed to control the interface distance of the heterostructures, such as the vacuum thermal annealing [49], diamond anvil cell [50], insertion of hexagonal BN dielectric layers [2], and nanomechanical pressure [51]. Importantly, the computational study performed here shall provide a design guideline for the experimentalist to further explore the engineering of interlayer distance as a useful experimental tuning knob to achieve the desired band alignments in BC\(_x\)N/P van der Waals heterostructures.

4. Conclusion

In summary, we investigated the structural, electronic and band alignment properties of the van der Waals heterostructures formed by the vertical stacking of BC\(_x\)N monolayer (\(x = 2, 6\)) and blue Phosphorene by using first-principles density functional theory simulation. An intrinsic type-II band alignments are formed in the BC\(_2\)N/P and BC\(_4\)N/P heterostructures. The band gap can be tuned and the band alignment can be switched between type-I and type-II by changing the interlayer distance via an external vertical strain. The proposed BC\(_x\)N and blue phosphorene monolayer shall offer a promising platform to study a large array of fundamental
phenomena, such as interfacial charge injection [52–54] and light–matter interactions [55], in atomically-thin materials. The results of this paper can be benchmarked by use the Heyd-Scuseria-Ernzerhof (HSE06) hybrid functional [56] or modified Becke-Johnson approach (mBJ) [57], which will require higher computational cost. Our results reveals the potential of a new class of van der Waals heterostructures composed exclusively of honeycomb lattices in optoelectronic applications, thus enriching the 2D material heterostructure family.

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