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Tunable electronic properties of graphene - fully hydrogenated boron nitride heterostructure: A van der Waals density functional study

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ABSTRACT

The structural and electronic properties of Gr/BN and Gr/H-BN-H heterostructures have been systematically investigated on density functional theory with van der Waals corrections. The results indicate that the band gap of Gr/H-BN-H is about 0.024 eV (without an electric field) and 0.412 eV (with a strong electric field). Moreover, the increase of band gap of Gr/BN and Gr/H-BN-H heterostructures does not lead an obvious drop in their carrier mobility. Meanwhile, Gr/H-BN-H heterostructure has a larger tunable range of band gap and carrier mobility than Gr/BN heterostructure. These electronic properties highlight graphene/BN potential applications in nanodevices with low energy consumption.

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1. Introduction

Since Geim et al. prepared single-layer graphene by micromechanical exfoliation in 2004, the graphene and two-dimensional materials has become one of the most rapidly developing areas of condensed materials [1]. Graphene with a hexagonal crystal structure, in virtue of its excellent electric, chemical and mechanical properties [2–4], becomes a competitive candidate for the next generation of semiconductor materials [5]. Actually, many experimental and theoretical studies have been conducted in order to explore the possibility of graphene being used to manufacture high-speed electronics [6]. On the one hand, graphene shows some excellent properties such as great charge carrier mobility ($1.5 \times 10^4 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ for a SiO₂-based sample [7] and $2 \times 10^5 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ for a suspended one [8,9]), high cut-off frequency [10] and stability as well as ambipolar electric field effect [1]. However, on the other hand, despite its extremely high carrier mobility, pristine graphene cannot be used for effective room temperature field effect transistors (FET) since its zero band gap. Ideal graphene, with obvious weaknesses of zero band gap as well as small on-off ratio, cannot be directly used to manufacture semiconductor components. Hence, how to tune the band gap of graphene has become an urgent and critical issue. Researchers have developed many methods to open the band gap of graphene. And these methods could be divided into two main categories depending upon whether they conserve the honeycomb structure of graphene [11]. Methods such as chemical functionalization and fabricating graphene nanoribbons [3] belong to category I, which destroy the honeycomb structure leading to the decrease of the carrier mobility in return, while oppositely band gap tailoring by applications of vertical

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external electric field, strain or substrate are external controls methods, belonging to category II [3,11], which the honeycomb structure of graphene as well as its high carrier mobility is well preserved. However, method of external electric field is feasible for bilayer graphene (BLG) but not for single layer graphene (SLG) [11]. Hence, it is quite desirable to find an effective way to tune the band gap of SLG without an obvious drop in its carrier mobility.

In fact, it is believed that the modified bilayer systems of graphene could play a vital role in the field of future nano-electronics. Recent development of techniques has realized to prepared graphene (Gr) on hexagonal boron nitride (BN) to form a van der Waals heterostructure, which not only has little lattice mismatch (about 1.7% [12]), but also can open the band gap with almost no drop in carrier mobility, even compared to suspended graphene, resulting from the atomically flat BN substrate being free from dangling bonds and charge impurities [13]. It is reported that the gapless Dirac spectrum is robust against small and moderate deformations, and the little lattice mismatch has very weak effect on the band structure of graphene, which has been proved in the previously reported ones [14,15]. The structure and electronic structure of graphene sandwiched between h-BN has been calculated by first principle method [11]. But generally, for the case of graphene, the electronic structure rapidly evolves with the number of layers, approaching the 3D limit of graphite at 10 layers [1]. Also, previous research shows the graphene - hexagonal boron nitride (Gr/BN) system and bilayer graphene are very closely related [16–22], so we prefer to research on the Gr/BN heterostructure and the influence of fully hydrogenated boron nitride on the Gr/BN heterostructure.

In this paper, the band gap and carrier mobility of Gr/BN heterostructure is tuned by an external electric field by using first principle calculations. Also, we try to apply the external electric field on the full hydrogenation of BN substrate (Gr/H-BN-H). These studies might provide us with more understanding of the Gr/BN and Gr/H-BN-H system, which is promising for future nanodevices.

2. Theoretical frame

Our DFT calculations were carried out by using the DMOL³ [23,24]. The generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof scheme (PBE) [25,26] is adopted for the exchange-correlation potential to optimize geometrical structures and calculate properties of Gr/BN heterostructures [27]. In order to take into account the contributions of the van der Waals (vdW) interactions between different layers, the DFT-D2 (D stands for dispersion) approach within the Grimme scheme is adopted for the vdW correction [28]. It has already been proved that Grimme method can correctly reproduce the structure properties of layered materials [29]. And the vdW methods could improve the determination of the distance d (interlayer spacing) and give a more accurate description of the dispersion forces between the atomic layers than PBE. This method has been successfully applied in previous studies of the interaction between antimonene [30], boron nitride [32] and silicene on graphene [31]. Moreover, double numerical atomic orbital plus polarization (DNP) is chosen as the basis set, with the global orbital cutoff 4.4 Å. DFT Semi-core Pseudopotentials (DSPP) are used for the core treatment. For graphene, single layer hexagonal boron nitride and Gr/h-BN heterostructure, the Brillouin zone is sampled by $16 \times 16 \times 1$ k -points for all structures in the geometry optimization (electronic) calculations, which brings out the convergence tolerance of energy of 1.0×10^{-5} Ha ($1 \text{ Ha} = 27.2114 \text{ eV}$), maximum force of $0.002 \text{ Ha}/\text{Å}$, and maximum displacement of 0.005 Å . Applying an electric field is carried out in DMOL³ module and it ranges from $-0.520 \text{ V}/\text{Å}$ to $+0.520 \text{ V}/\text{Å}$. Moreover, we also consider the cell size effect of band gap on the heterostructures. After simulation, we found that band gap on the heterostructures almost didn't change as size of supercell increase. Therefore, 2×2 supercell is used to calculate the band structure below. Meanwhile, it is worth noting that there still exists some discrepancy between theory and experiment in predicting numerically accurate values of band gaps for heterostructure, partly due to the choices in the exchange–correlation functional and the inclusion of many-body effects [33,34].

Binding energy (E_b) can be used to assess the structural stability of the heterostructure system. When graphene and BN are combined to form a single-layer heterostructure, the binding energy (E_b) of the heterostructure is defined by the following formula:

$$E_b = (E_{\text{Graphene}} + E_{\text{BN}}) - E_{\text{heterostructure}} \quad (1)$$

where, $E_{\text{heterostructure}}$, E_{Graphene} and E_{BN} are respectively the energy of heterostructure system, graphene and boron nitride which have the same lattice parameters. According to this definition, the positive value of E_b means heterostructure system to stabilize binding, and the greater value of E_b is, the more stable binding of the heterostructure system is.

3. Results

As shown in Fig. 1 and Table 1, Gr/BN heterostructures are stacked by monolayer graphene and hexagonal boron nitride. There are five different initial stacking structures: B atom and N atom simultaneously locate just above the C atoms (T), B atom locates above the midpoint of C–C bond (B_B) or N atom locates above the midpoint of the C–C bond (B_N), B atom is positioned above the center of C atom six-membered ring (H_B) or so does N atom (H_N). Meanwhile, Gr/H-BN-H is also shown in Fig. 1f. After geometry optimization, we found that the B_N and B_B were unstable and then the structure of the B_N will transform to the structure of H_B and the structure of B_B will transform to the structure of H_N finally. Hence, B_N and B_B are not considered in the

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