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Stacking nature and band gap opening of graphene: Perspective for optoelectronic applications

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ABSTRACT

Using first principles density functional theory calculations, we have performed geometrical and electronic structure calculations of two-dimensional graphene(G) sheet on the hexagonal boron nitride (*h*-BN) with different stacking orders. We found that AB stacking appears as the ground state while AA-stacking is a local minima. Band gap opening in the hybrid G/*h*-BN is sensitive to the interlayer distance and stacking arrangement. Charge redistribution in the graphene sheet determined the band gap opening where the onsite energy difference between carbon lattice atoms of G-sheet takes place. Similar behavior can be observed for the proposed h-BN/G/h-BN tri-layer system. Stacking resolved calculations of the absorptive part of complex dielectric function and optical conductivity revealed the importance of the proposed hybrid systems in the optoelectronics.

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1. Introduction

Graphene, a monolayer carbon allotrope has attracted excessive efforts in determining its physical properties for potential applications in nanodevices [1]. The gapless excitation due to its two linear bands at Fermi level allows its high carrier mobility and hence remarkable electronic properties [2]. Although, having magnificent physical properties, the gapless nature of graphene limits its practical implantation in high speed transistor applications. Since then, the opening of energy gap in graphene became a focus of the research community and several attempts have been put forward for this purpose.

Numerous methods have been employed for opening the band gap in graphene, but the diminishing intrinsic properties become a prominent barrier. These methods encompassed molecular adsorption, hydrogenation and defect generations in the graphene structure [3–9]. The graphene-substrate method involves bandgap opening of graphene through preparing a hybrid structure of graphene over a substrate. This fabrication method serves as the easiest of all the adopted procedures [9–11]. Epitaxially grown graphene over the silicon-carbide substrate has shown the opening of band gap in due of the strong interaction between the layers [11]. Though, the intrinsic symmetry of graphene destroyed, this method stimulated the attention of the researchers to opening the energy gap in graphene while keeping the graphene intrinsic properties [12–17]. Of the distinct interest, the insulating hexagonal boron-nitride (h-BN) that weakly couples graphene keeping the highest mobility [18], ballistic transport [17] and fractional Hall effect [18], ever registered for graphene over any substrate.

Many theoretical investigations and simulations studies have been performed to study the band gap opening of graphene over the h-BN substrate through variations in stacking in hybrid system [16–25]. These investigations covered either crafting of bilayer or tri-layer graphene and boron nitride single sheets for band gap of single layer graphene (SLG). On the other hand, the graphene/h-BN hybrid system inevitably involves the modifications in the geometric configurations and the parent optical absorption, which are of crucial importance for material characterization in fabricating nano-devices. Earlier studies put forward the electronic properties of graphene over different substrates and found different extent of band gap opening for different stacking order, but the underlying mechanism is still an open issue.

In this study, we have considered the different stacking order for graphene/h-BN bilayer system for elucidating the geometrical, orbital and charge orders of graphene(G) layer in the hybrid system as function of the bilayer G/h-BN interlayer distance. Based on promising results from bilayer system; we have proposed tri-layer

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h-BN/G/h-BN (ABA) arrangement that exhibit assertive electronic results. The study is then accompanied by the respective optical absorption due to the above characters in different stacking schemes.

2. Computational method

In this work, we performed first-principles full potential linearized augmented plane wave (FP-LAPW) [26] calculations based on the density functional theory (DFT) [27,28] which is implemented in the Wien2k package [29]. The bilayer and tri-layered two dimensional (2-D) atomic structures are constructed in xy-plane keeping large (15 Å) vacuum along *z*-axis to prevent the interaction between adjacent periodic layers. In the FP-LAPW method, the exchange-correlations are treated by generalized gradient approximation proposed by Perdew, Burke and Ernzerhof (PBE) [30]. Monkhorst–Pack *k*-mesh of $29 \times 29 \times 1$ was used for geometrical optimization and self consistent field calculations to generate the accurate optical absorption of G/h-BN hybrid system. All designed structures are relaxed till the value the forces less than 0.01 eV/Å and reaching the total energy criterion of 0.0001 eV. The absorptive part of the complex dielectric function [31,32] is computed to uncover the interband optical absorption and optical conductivity of the understudy systems.

3. Results and discussion

To reveal the physics of graphene over h-BN substrate, two stacking models were considered. The first one involves stacking patterns shown in Fig. 1(a), where in AA stacking, the carbon hexagon is directly placed over the BN hexagon. The second model involves AB stacking which was designed in two configurations where one C-atom is directly placed over N (see Fig. 1(b)) or B (Fig. 1(c)) atom and the 2nd C-atom is positioned over the center of BN hexagon. We have taken three hybrid systems which were relaxed to stable structures and found the equilibrium interlayer distance of 3.28 Å, 3.41 Å and 3.35 Å for structures shown in Fig. 1 (a)–(c) respectively. Total binding energy calculations has been carried out to escort with the previous theoretical and experimental reports [14,15] which showed that AB-stacking is ground state while AA-stacking is the local minimum. Calculated binding energy difference between AB(C/B) and AA stackings is −0.0141 eV. On other hand, this difference is between AB(C/B) and AB(C/N) is −0.0037 eV, revealing the AB(C/B)-stacking as ground state. In the relaxed equilibrium structures, the C–C and B–N bond lengths are 1.475 Å and 1.476 Å in AA-stacking, 1.537 Å and 1.583 Å in AB(C/N) stacking and 1.532 Å and 1.535 Å in AB(C/B) stacking. The hexagonal C–C–C and B–N–B angles are 119.96° and 119.95° in AA-stacking, 119.02° and 120.15° in AB(C/N) stacking and 120.7° and 119.42° in AB-stacking. Departure from the ideal hexagonal angle in AA-stacking can be attributed to the vertical attraction between corresponding B and C atoms due to valence band enhanced overlapping of BN layer with π states of graphene sheet [33]. The deviations in the magnitudes of the bond lengths and hexagonal angles from the ideal system in both layers indicate the possible changes in the related physical properties. Motivated by the bilayer system, we have designed the tri-layer ABA-stacking system as given in Fig. 1(d)–(g). The structure relaxation to the equilibrium ABA composition determined the 3.26 Å, 3.23 Å, 3.22 Å and 3.22 Å interlayer G-BN distances for tri-layer ABA structures shown in Fig. 1(d)–(g). Also, the in-plane geometry traumatized such that the inter-atomic direct vertical distance between C and B decreased.

The effect of stacking in the G/BN hybrid system on the band gap of graphene is studied via the calculations of the band structure for various interlayer separations. The calculated band structure of G/BN bilayer system of considered structures at equilibrium interlayer distances is shown in Fig. 2(a, b). The calculated energy gap for the AA-stacking system is 140 meV and 30 meV for both the AB stacking structures at equilibrium interlayer distance. Decrease in interlayer distance induces the increase in the band gap of hybrid system while the maximum energy gaps of 581 meV, 353 meV and 340 meV are predicted for the lowest interlayer distance (2.65 Å) used in our calculations. To take a clearer view, we have plotted first order exponential fit to the band gap as a function of the interlayer distance as shown in Fig. 3(a). The figure clearly shows that for a given interlayer distance, the magnitude of band gap for AA-stacking is always greater than that for AB-stacking, while nearly the same for both structures in AB-stacking. Following the bilayer structures, we have computed the band structures of tri-layer (ABA) systems as discussed earlier. The band gap opening in the structures of Fig. 1(c)–(g) was observed while

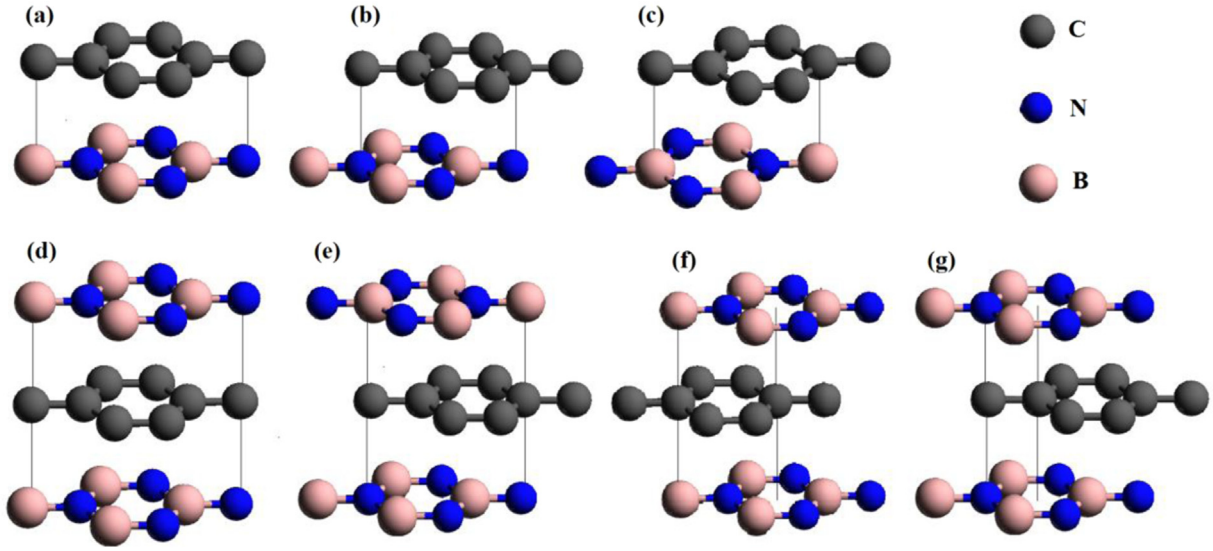

Fig. 1. (Color online) The considered hybrid structures (a) AA-stacking (b) AB(C/N) stacking (one carbon atom directly over the nitrogen atom and other one is above the center of BN hexagon), (c) AB(C/B) stacking (one carbon atom directly over the boron atom and other one is above the center of BN hexagon), (d) ABA-stacking (B–C–B, N–C–N), (e) ABA-stacking (B–C–N, H–C–H), (f) ABA-stacking (B–C–B, H–C–H) and (g) ABA-stacking (N–C–N, H–C–H), where "H" stands for the center of BN-hexagon.

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