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Electronic band structure of Graphene/h-BN Hetero junction: A Tight Binding Model Study

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Abstract. We address here the electronic band dispersion of graphene/h-BN hetero junction in a transverse applied electric field. The system is described by kinetic energy with nearest neighbor electron-hopping with hopping energy t_1 and gate potential V across the two layers. The electron Green's functions are calculated by Zubarev's Green's function technique and electron band dispersion is found by equating the denominator of the Green's function to zero. It is observed that the graphene/h-BN system exhibits the band dispersion, where the two bands form a small gap and other two bands form a large gap near the Dirac point. For the application in the electronic devices, these two bands can be modified by the transverse hooping integral and the external biasing potential representing the suitable impurity effects.

Keywords. Graphene/h-BN system, Tight-binding method, Green's function, Electron band dispersion

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1. Introduction

Graphene, a two-dimensional monoatomic layer of carbon atoms, which has honeycomb structure of a sp^2 hybridized carbon network, has attracted huge attention due to its high carrier mobility and is considered to be an ideal material for carbon based nano-electronics [1,2]. In the reciprocal space of graphene, two bands with p_z character cross at the Fermi level and the absence of gap is due to the equivalence of the two carbon sub-lattices, rendering graphene as a zero

band-gap semiconductor. If the two sub-lattices are made in-equivalent, significant modifications in the electronic properties of the semi-metallic graphene can be anticipated [3].

In Bernal stacking bilayer graphene (BLG), the opening and external tuning of energy gap between valence and conduction bands show the largest potential for logic applications[4]. In contrast to single layer graphene (SLG), bilayer graphene has massive Dirac fermions with an effective mass, $m^* \approx 0.03m_e$, where m_e is the bare electron mass [5]. Since the exceptional conical dispersion is not preserved, an important question, "whether it is possible to open a band gap, while retaining the extraordinary electronic properties of SLG?", arises. Recently, several proposals of band gap engineering, including surface bonding (graphane), isoelectronic co-doping with boron, nitrogen, or alternating electrical or chemical environment (by using Li and F atoms) have been reported [6]. Hexagonal boron nitride (h-BN) is a promising material for laser devices because of its large direct band gap in the ultraviolet region [7]. This property of h-BN is of immense importance in the field of optical storage, photo-catalysis, sterilization, ophthalmic surgery and nano-surgery. Recently, Graphene/h-BN hybrid system has attracted extensive attention due to its electronic properties, and analogy with graphene, which makes graphene/h-BN system suitable for graphene based device design. When graphene is grown on h-BN substrates, its electron mobility rises up to ten times higher than the graphene grown on SiO_2 substrates [8]. To engineer the band gaps in graphene, the graphene/h-BN hybrid system is a promising hetero structure for the electronic device applications [9]. Due to close lattice matching, carbon and boron nitride mixed structures show various exceptional physical properties. Giovannetti et al. [10] have studied the most stable configuration in graphene/h-BN hybrid system, where one carbon atom is above the boron atom while other carbon atom is above the centre of the boron nitride ring. They observed a band gap energy of the order of 53 meV at the K point, due to the graphene-substrate interaction in the van der Waals hetero structure, with the help of density functional theory (DFT) calculations.

Here, we describe the formalism and the minimal tight-binding model in section 2, the calculation of the electron Green's function and expression for self-consistent calculation for electron occupancies of graphene at both sites for each spin in section 3. We present our results and discussion and finally conclusion in section 4.

2. A minimal tight-binding model Hamiltonian

The Hamiltonian for externally biased monolayer h-BN at bottom of the hybrid system is represented as

$$H_1 = \sum_{k,\sigma}\left\{\left(E_{B1} + \frac{V}{2}\right) a^{\dagger}_{1k,\sigma} a_{1k,\sigma} + \left(E_{N1} + \frac{V}{2}\right) b^{\dagger}_{1k,\sigma} b_{1k,\sigma}\right\} - t_1 \sum_{k,\sigma}\left(\gamma_1(k)\, a^{\dagger}_{1k,\sigma} b_{1k,\sigma} + \gamma_1^{*}(k)\, b^{\dagger}_{1k,\sigma} a_{1k,\sigma}\right) \quad (1)$$

Similarly, the Hamiltonian externally biased monolayer graphene on top of the hybrid system is represented as

$$H_2 = \sum_{k,\sigma}\left\{\left(E_{C1} - \frac{V}{2}\right) a^{\dagger}_{2k,\sigma} a_{2k,\sigma} + \left(E_{C2} - \frac{V}{2}\right) b^{\dagger}_{2k,\sigma} b_{2k,\sigma}\right\} - t_{11} \sum_{k,\sigma}\left(\gamma_1^{*}(k)\, a^{\dagger}_{2k,\sigma} b_{2k,\sigma} + \gamma_1(k)\, b^{\dagger}_{2k,\sigma} a_{2k,\sigma}\right) \quad (2)$$

The Hamiltonian [11] for interlayer interaction between h-BN and graphene can be expressed as

$$H_{\perp} = -t_{\perp} \sum_{k,\sigma}\left(\gamma_{\perp}(k)\, a^{\dagger}_{1k,\sigma} b_{2k,\sigma} + \gamma_{\perp}^{*}(k)\, b^{\dagger}_{2k,\sigma} a_{1k,\sigma}\right) \quad (3)$$

Hence, the net Hamiltonian for this hybrid system can be written as;

$$H = H_1 + H_2 + H_{\perp}$$

3. Calculation of Green's functions and band dispersion Graphene/ h-BN bilayer system

In order to calculate the physical parameters, we calculate the four coupled electron Green's functions involving electrons of h-BN at boron-site and the Green's functions are defined as;

$$A_1(k,\omega) = \ll a_{1k,\sigma}\,;\, a^{\dagger}_{1k,\sigma} \gg_{\omega}, \qquad A_2(k,\omega) = \ll b_{1k,\sigma}\,;\, a^{\dagger}_{1k,\sigma} \gg_{\omega}$$

$$A_3(k,\omega) = \ll a_{2k,\sigma}\,;\, a^{\dagger}_{1k,\sigma} \gg_{\omega}, \qquad A_4(k,\omega) = \ll b_{2k,\sigma}\,;\, a^{\dagger}_{k,\sigma} \gg_{\omega}$$

Employing Zubarev's Green's function technique, the total Hamiltonian is solved for these Green's functions as well as the coupled equations. The solution of the coupled equations for the Green's functions $A_1(k, \omega)$ is given as

$$A_1(k,\omega) = \frac{\left(\omega - E_{N1} - \frac{V}{2}\right)}{2\pi}\left[\frac{\left(\omega - \bar{E}_{C1} + \frac{V}{2}\right)\left(\omega - \bar{E}_{C2} + \frac{V}{2}\right) - t_{11}^2|\gamma_1(k)|^2}{|D(\omega)|}\right] \quad (4)$$

The $|D(\omega)|$ appearing in the denominator of the Green's function given in equation (4) is written as;

$$|D(\omega)| = a\omega^4 + b\omega^3 + c\omega^2 + d\omega + e \quad (5)$$

where, the coefficients of different orders of ω in the quartic relation of $|D(\omega)|$ are written in terms of physical parameters of the graphene-h-BN bilayer system. Equating $|D(\omega)|$ to zero, one can obtain the electron band dispersion energy of the graphene-h-BN bilayer system, i.e., $|D(\omega)| = 0$. Since this equation is quartic in ω, it is not possible to calculate the band dispersion energy analytically. Therefore, we have numerically solved the quartic equation, taking 100×100 grid points of the electron momentum in the plane of the bilayer system, and obtained three quasi-particle band dispersion energies denoted as $\omega_{\alpha k}(\alpha = 1 - 4)$. Then we have solved the Green's function $A_2(k, \omega)$, $A_3(k, \omega)$, and $A_4(k, \omega)$. Similarly, we can define the Green's functions involving electrons at nitrogen site and both site of carbon.

4. Results and Discussion

Before numerical computation, we have scaled the physical parameters with respect to the nearest neighbor electron hooping interaction $\boldsymbol{t_1}$. The dimensionless physical parameters are the nearest neighbor hooping integral $\boldsymbol{t_1}$, transverse hooping integral $\boldsymbol{t_p} = \frac{\boldsymbol{t_\perp}}{\boldsymbol{t_1}}$. The external biasing potential $\boldsymbol{v} = \frac{\boldsymbol{V}}{\boldsymbol{t_1}}$, the site energies of carbon $\boldsymbol{E_{c1} = 0}$, $\boldsymbol{E_{c2} = 0}$ and that of Boron = $\frac{\boldsymbol{+E_b}}{\boldsymbol{t_1}}$, nitrogen = $\frac{\boldsymbol{-E_N}}{\boldsymbol{t_1}}$. The band dispersion energy is numerically computed and plotted taking band energy along y-axis and electron momentum along x-axis. The continuous lines represent the four dispersion bands for ideal bilayer graphene, where the inner two bands show zero band gap and outer layers show a small band gap at k-point. The dotted lines show four bands form ideal bilayer h-BN systems with very small gap due to the two inner bands, while a large gap of the order of $\boldsymbol{5\ eV}$ due to outer bands at k-point implying its insulating character. Further, we observe large band gaps at **Γ** points for both the above two cases. When graphene

is placed on the substrate like h-BN layer, the resultant band dispersion shown in figure 1 and complete new scenario represent by the four bands shown by dashed-dot lines. The outer two bands form a large band gap at the k-point and a much larger band gap at **Γ** point, while the inner two bands exhibits very small band gap at the k-point and relatively larger gap at the **Γ** point. Further the inner two bands are compressed drastically. This type of band formation at the graphene/h-BN hetero-junction are useful for electron device application.

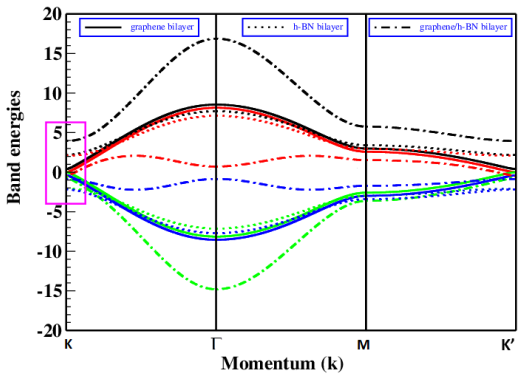

Fig. 1. Plot of band energies vs. momentum (k) for different bilayer systems i.e. bilayer graphene, bilayer h-BN and graphene/h-BN Hetero junctions at $\boldsymbol{\Gamma - Point}$.

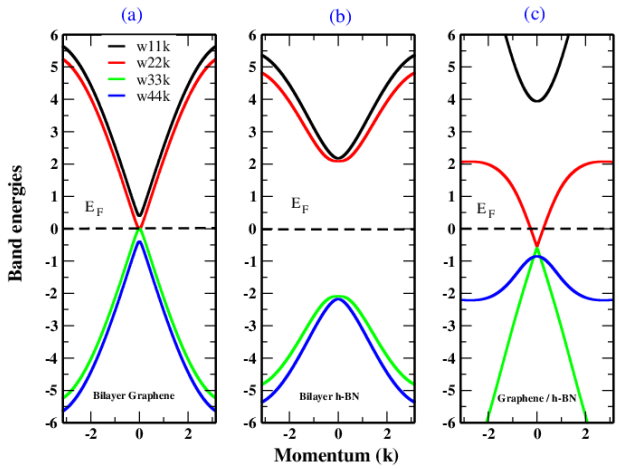

Fig. 2. Plot of band energies vs. momentum (k) for different bilayer systems i.e. bilayer graphene, bilayer h-BN and graphene/h-BN Hetero junctions at K-Point.

We have plotted the band energy vs. electron momentum plot at the Dirac point as shown in figure 2 (a, b, c). The figure 2(a) shows the band dispersion of ideal bilayer graphene with zero band gap at the k-point. Similarly the figure 2(b) shows the larger band gap across the k-point for the ideal bilayer h-BN system representing its insulating character. The figure 2(c) shows the band dispersion for the graphene on h-BN system. Here we observe that the two bands near the k-point form a small gap, while the outer two bands form a large gap. These two gaps can be engineered near the Dirac point by varying the transverse hooping integral as well as the transverse external biasing potential according to the requirements of the device application.

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