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Effect of an out-of-plane cross connection on the electronic transport of zigzag graphene nanoribbon

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ABSTRACT

Electronic transport properties of out-of-plane graphene nanoribbon intersections have been investigated by using computational method. The inter-distance between two graphene nanoribbons is found to affect the transport properties strongly and its affection can be neglected for larger ones, even under an external bias. Wider graphene nanoribbons will bring stronger interaction into the system, and result in more transmission dips. Moreover, the stacking configuration between two graphene nanoribbons is found to be crucial for the electronic transport under an external bias, as it can affect the electronic transport strongly near the charge neutral point.

1. Introduction

Many efforts have been devoted into designing and fabricating practical graphene-based nanoelectronic devices since graphene has been prepared experimentally [1–3]. In graphene-based nanoelectronics, graphene usually appears in the form of graphene nanoribbon (GNR). GNR has many unique properties, such as energy gap dependence of widths [4–7] and ballistic transport [8,9]. Especially, zigzag graphene nanoribbon (ZGNR) exhibits great metallic behavior when it has no mirror plane [10].

Based on some theoretical and experimental works, GNR will be used widely in graphene-based nanoelectronics [11,12]. By the development of nanoelectronics, graphene circuits inevitably become complex and the GNRs may connect with each other in many different configurations [8]. Out-of-plane GNR intersection is a kind of possible connection structure and can be obtained from an aligned carbon nanotubes (CNTs) array [13]. Recently, an out-of-plane GNR network has been studied theoretically and the simulation results demonstrate that the angle between GNRs affect the transport strongly [14]. In this present work, an out-of-plane GNR intersection which constructs from one zigzag graphene nanoribbon (ZGNR) and one armchair graphene nanoribbon (AGNR) is studied by computational method. The transport properties of out-of-plane GNR intersection were calculated and the effect of inter-distance, width of AGNR, external bias and stacking configurations is considered further.

Our simulation results show that no matter the out-of-plane GNR intersection is under an external bias or not, inter-distance between two GNRs is found to affect the transport properties strongly and this affection can be neglected for larger inter-distances. Small inter-distances cause dips in the transmission spectrum while larger ones cannot. Wider GNRs bring a stronger interaction to the system, result in more transmission dips. Especially, transmission decreases appear near the charge neutral point because of an external bias. Moreover, the stacking configuration between the two graphene nanoribbons is found to be crucial for the electronic transport under an external bias, as it can affect the transport strongly near the charge neutral point.

2. Calculating methods

The structure we studied is shown in Fig. 1. This out-of-plane intersection is patterned from AB-stacking graphene bilayer. It constructs from one ZGNR and one AGNR, which are vertical to each other. The ZGNR contains $N_Z = 3$ zigzag chains along its width direction, while the AGNR contains $N_A = 6$ dimmer chains. Both of these two GNRs are saturated by H atoms on the edges to eliminate the dangling bonds.

Atomistix Toolkit code was used to calculate the electronic transport properties of out-of-plane GNR intersections [15,16]. The

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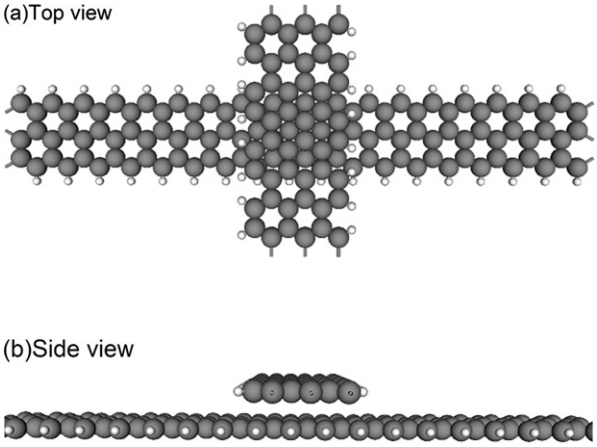

Fig. 1. Ball and stick model of GNR out-of-plane cross connection shape. The structure is constructed by one $N_Z = 3$ ZGNR and one $N_A = 6$ AGNR. Both GNRs are saturated by H atoms on the edges to eliminate the dangling bonds.

local-density approximation (LDA) is chosen for the exchange correlation functional. A single-zeta plus polarization orbital basis set is used to expand the wave function. The mesh cutoff energy for the integration in the real space grid is chosen as 150 Ry, and the Brillouin zone is integrated with $1 \times 1 \times 100$ k-points Monkhorst–Pack grid. The quantum transmission spectrum is calculated in the theoretical frame of Green's function:

$$T(E) = \mathrm{Tr}\left[t^{\dagger}t\right] = \mathrm{Tr}\left[\Gamma_L G^r \Gamma_R G^a\right], \tag{1}$$

where t is the transmission matrix. G^r and G^a represent the retarded and advanced Green's function in the scattering region respectively. $\Gamma_{L(R)}$ is the coupling matrix between the left (right) electrode and the scattering region. Above three matrices can be represented as:

$$G^r = (ES - H - \Sigma_L - \Sigma_R)^{-1}, \tag{2}$$

$$G^a = G^{r\dagger}, \tag{3}$$

$$\Gamma_{L(R)} = i\left(\Sigma_{L(R)} - \Sigma^{\dagger}_{L(R)}\right), \tag{4}$$

here $\Sigma_{L(R)}$ is the corresponding self-energy term. The conductance G can be evaluated by following formula:

$$G = G_0 T(E_f), \tag{5}$$

where $G_0 = 2e^2/h$ is the conductance quantum.

3. Results and discussions

3.1. Effect of the inter-distance between individual GNRs

We calculate the transport properties of an isolated ZGNR containing 3 zigzag chains ($N_Z = 3$), and the transmission spectrum is shown in Fig. 2(a). It exhibits good metallic behavior, which makes it suitable for conducting wires. This metallic behavior comes from the asymmetry of the $N_Z = 3$ ZGNR [10].

Transport properties of an out-of-plane intersection of two GNRs (Fig. 1) containing 3 zigzag chains (ZGNR with $N_Z = 3$) and 6 dimmer chains (AGNR with $N_A = 6$) has been investigated here. The inter-distance is set to be a series of values ranging from 3.0 to 5.0 Å. Zero-bias transmission spectrum of the ZGNR with $N_A = 6$ cross connection was calculated and shown in Fig. 2(a). When L is larger than 4.0 Å, the effect of top AGNR can be neglected. And when L becomes smaller, interaction between two GNRs becomes stronger. This interaction results in conductance dips in the transmission spectra at $E = -0.39$, 0.10, and 0.60 eV near the charge

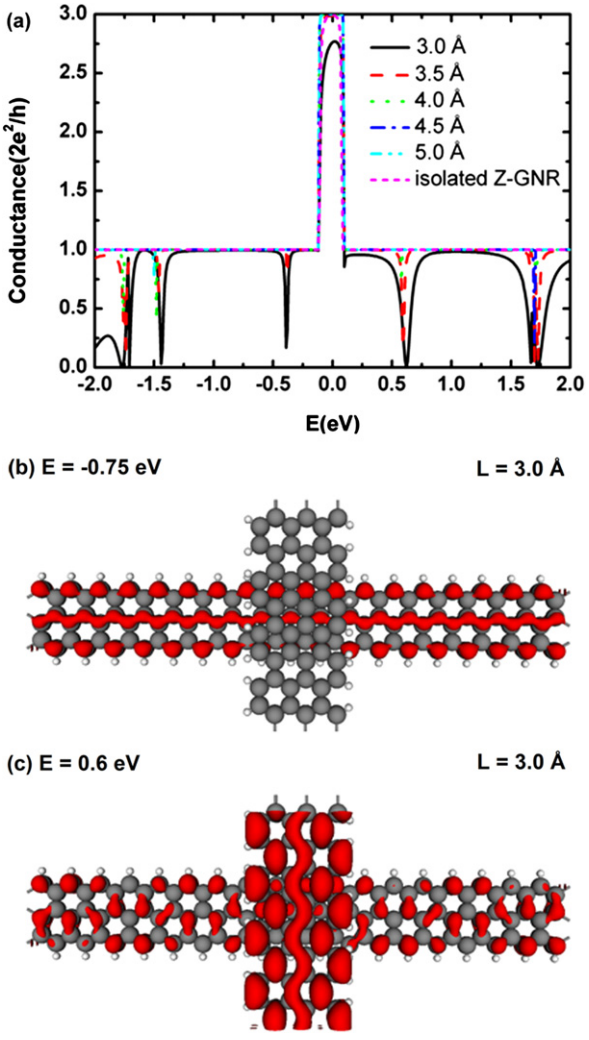

Fig. 2. (Color online.) (a) Zero-bias transmission spectra of $N_Z = 3$ ZGNR with out-of-plane cross connections for different inter-distances (L). Zero energy is set to be the Fermi level and the same as following. For $L = 3.0$ Å case, LDOSs at $E = -0.75$ and $E = 0.6$ eV are shown in (b) and (c), respectively. The corresponding isovalues of them are set to be 0.01 e/Å^3.

neutral point (Fig. 2(a)). Spatially localized density of states (LDOS) of the $L = 3.0$ Å GNR cross connection structure was calculated. The LDOSs at $E = -0.75$ and 0.6 eV are shown in Figs. 2(b) and 2(c) respectively. These two energy points correspond to the energy with the transmission of $1.0G_0$ and the energy with a dip, respectively. At $E = -0.75$ eV, the out-of-plane GNR cross structure exhibits rich edge states. This GNR intersection structure has the same electron distribution to the corresponding isolated ZGNR (not shown). The added top AGNR does not alter the conductance at $E = -0.75$ eV. But for $E = 0.6$ eV, the conductance exhibits a sharp decrease compared to the isolated $N_Z = 3$ ZGNR. From Fig. 2(c), there are rich states on the top AGNR at $E = 0.6$ eV. Due to quantum interference between AGNR and ZGNR, resonance states formed. The states of LDOS, especially the edge states, in ZGNR are not continuous anymore due to the interaction between individual GNRs, compared with that in Fig. 2(b). So the sharp decrease of transmission appears. The same conclusion can also be found for other energies with transmission dips, e.g., −0.38 eV.

The effect of width of AGNR on the transport properties of out-of-plane has been investigated too. The width of ZGNR is fixed to be $N_Z = 3$ while the width of AGNR is increased to $N_A = 8$ and $N_A = 10$. The corresponding conductance spectra of ZGNR are shown in Figs. 3(a) and 3(b) respectively. The out-of-plane GNR

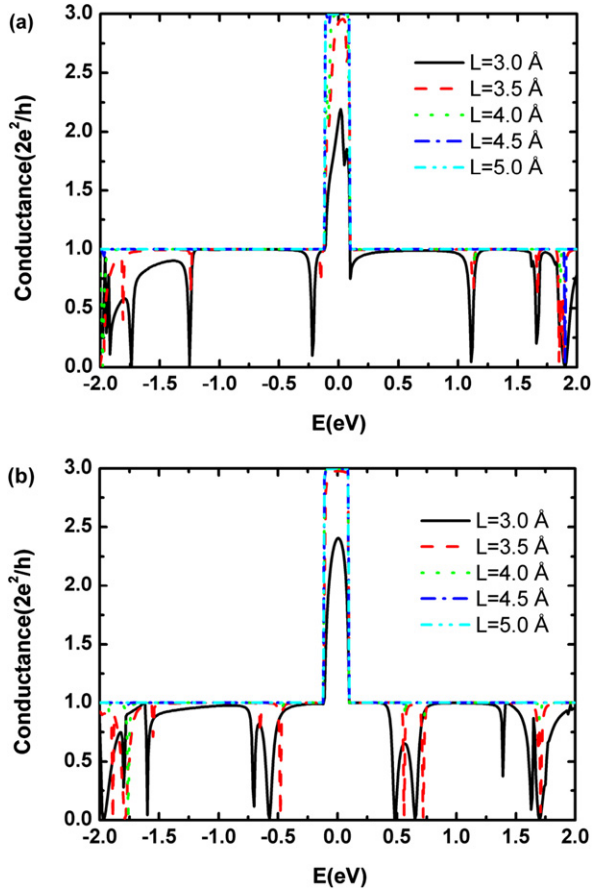

Fig. 3. (Color online.) (a) Zero-bias transmission spectra of $N_Z = 3$ ZGNR with $N_A = 8$ AGNR out-of-plane cross connection structures for different inter-distances. (b) Zero-bias transport spectra of $N_Z = 3$ ZGNR with $N_A = 10$ AGNR out-of-plane cross connection structures for different inter-distances.

intersections with large inter-distance (L) exhibit similar conductance spectrum like that of $N_A = 6$ case in Fig. 2(a). But when L becomes smaller, more sharp dips appear in the transmission curves. These dips suggest that more resonance states formed.

3.2. Effect of an external bias

A finite external bias is added to the ZGNR part of out-of-plane GNR system along the length direction and the electronic transport has been studied. This external bias is set to be 1.0 V. The 1.0 V-bias transport properties of the out-of-plane GNR cross connection in Fig. 1 are calculated and the conductance spectra are shown in Fig. 4(a). For a large L, such as 5.0 Å, it shows a good metallic behavior (Fig. 4(a)). The transmission curve is nearly a horizontal line. But when L becomes smaller, transmission dips appear (Fig. 4(a)) because of the interaction between two GNRs and the 1.0 V external bias. We take the $L = 3.0$ Å case as an example to study. The projected density of states (PDOS) of the out-of-plane system under the bias of 1.0 V is calculated, shown in Fig. 4(b). Interestingly, each maximum value in the PDOS corresponds to the minimum in the $L = 3.0$ Å transmission spectrum in Fig. 4(a). This clear correspondence demonstrates that the GNR cross connection system has rich density states at these energy points, but these states are quite localized and could not contribute to the conductance. Thus the transmission dips appear. To further confirm this physical picture, we plot the spatial LDOSs at four maxima near charge neutral point, −0.51, −0.38, −0.10 and 0.48 eV (Figs. 4(d)–4(g)). Each case shows the distribution of electron states in real space. None of them distributes throughout the whole ZGNR, so the states do not contribute to the conductance and transmission dips appear. Furthermore, we calculated the currents of the system under the bias of 1.0 V for different inter-distances (Fig. 4(c)). Apparently, the top AGNR has little effect on the transport of ZGNR when L is larger than 4.0 Å.

3.3. Effect of stacking configuration

For practical application, the ideal stacking configuration between individual GNRs cannot always be achieved. When the top AGNR translates a certain distance along the length direction of ZGNR, different stacking types will generate. The effect of the different stacking configurations has been investigated consequently. L is fixed to be 3.0 Å and the AGNR is translated a certain distance along the longitudinal direction of ZGNR. The cell-length along the length direction of ZGNR is $a = 2.461$ Å. We divided it into four parts, and translate the top AGNR in $a/4$, $2a/4$, and $3a/4$ (Fig. 5(a)). Zero-bias and 1.0 V-bias conductance spectra of these

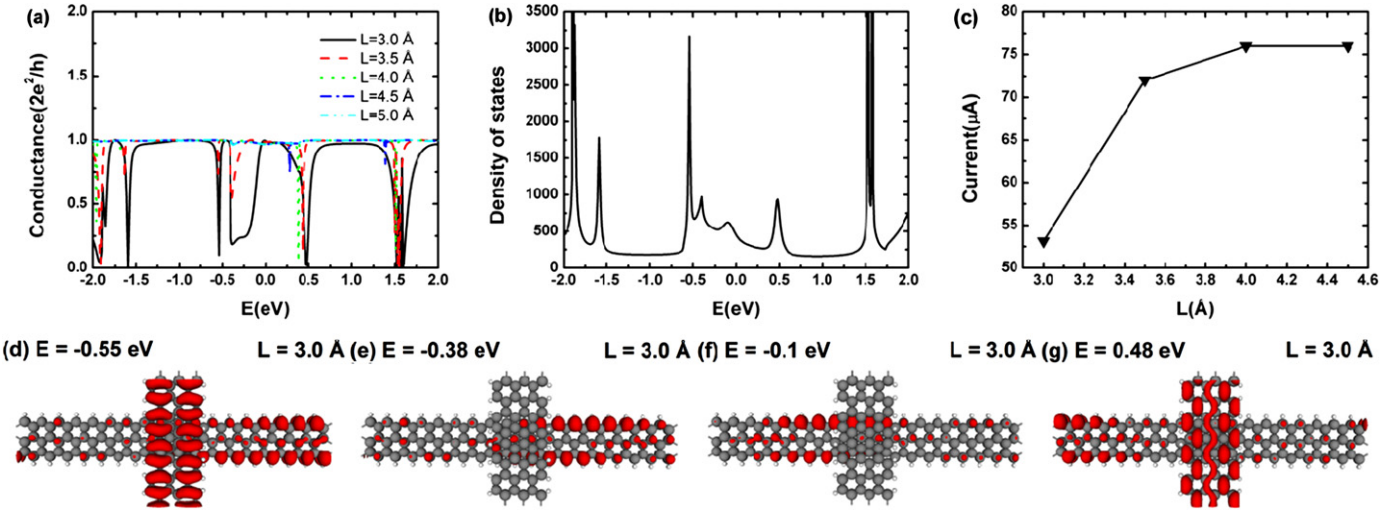

Fig. 4. (Color online.) (a) 1.0 V-bias transmission spectra of the ZGNR with AGNR out-of-plane cross connections for different inter-distances. (b) PDOS of ZGNR part under the bias of 1.0 V. (c) Currents for different inter-distance cases under the bias of 1.0 V. (d)–(f) LDOSs of the system for $L = 3.0$ Å case at the energies of −0.51, −0.38, −0.10 and 0.48 eV, respectively. All the isovalues of these four LDOSs are set to be 0.03 $e/\text{Å}^3$.

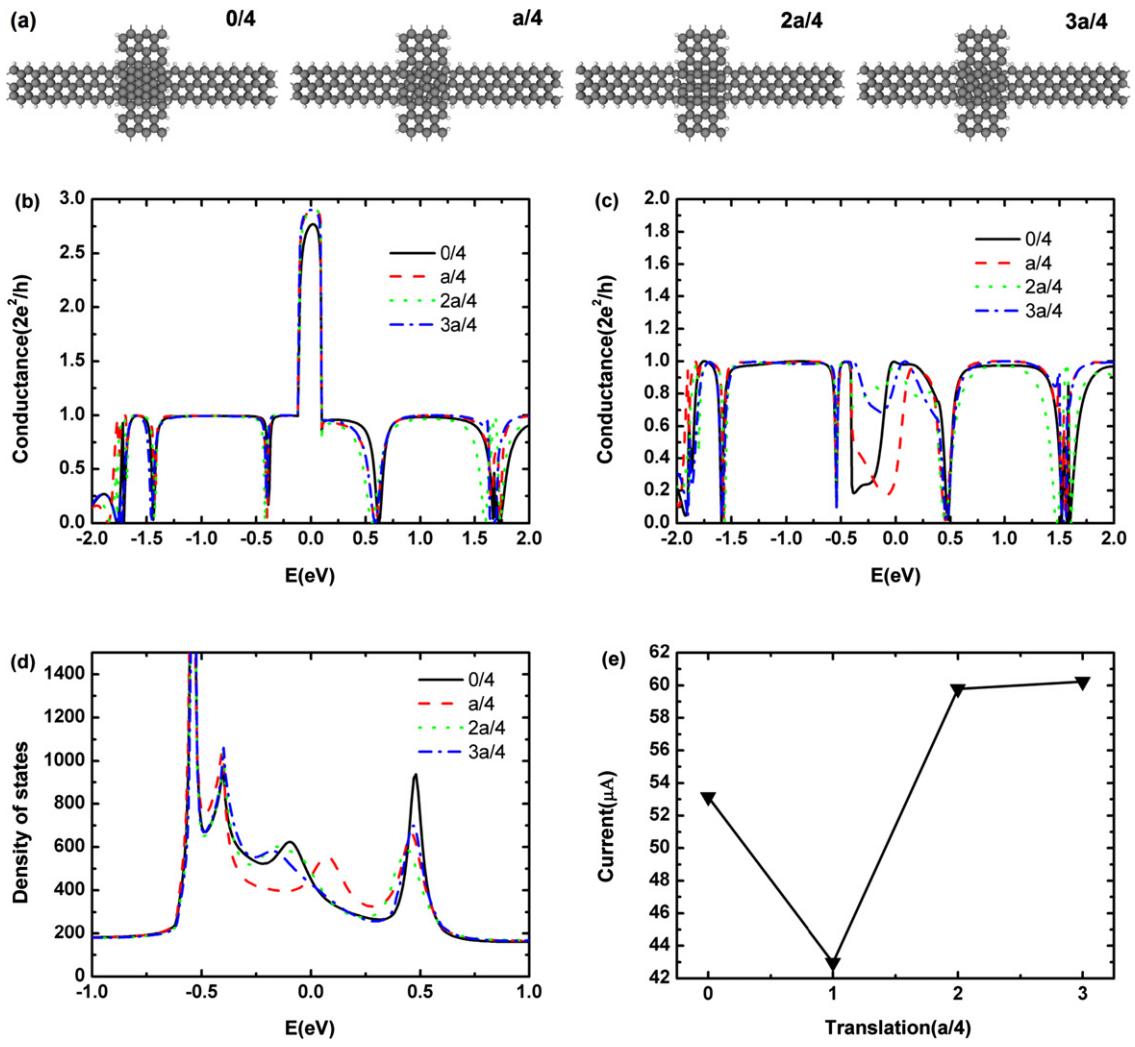

Fig. 5. (Color online.) (a) Ball and stick model for four kinds of stacking structures ($L = 3.0$ Å). (b) Zero-bias transmission spectra of the four structures in (a). (c) 1.0 V-bias transmission spectra of these four cases. (d) PDOS of cross connection for these four cases under the bias of 1.0 V. (e) Currents for the four cases under the bias of 1.0 V.

different stacking type structures are present In Figs. 5(b) and 5(c) respectively. Zero-bias conductance spectra of these four different stacking structures exhibit very similar curve shapes. Transport properties along the ZGNR are not sensitive to the stacking type because that both the cross area and the distance between two GNRs alter a little by the different stacking types. But the 1.0 V-bias conductance spectra of these four stacking structures are quite different near the charge neutral point. Interestingly, the peaks in the PDOS of ZGNR (Fig. 5(d)) correspond to the dips in conductance (Fig. 5(c)). That means the external bias has strong and different effects on the bilayer part for different stacking configuration. In addition, the 1.0 V-bias currents of these four different stacking structures are shown in Fig. 5(e). The current exhibits large oscillation when the AGNR translates. This result is helpful for the circuit design and the application of GNR.

4. Conclusions

Out-of-plane GNR cross connection is an elemental structure in graphene-based nanoelectronics. When an isolated conducting ZGNR is combined with an out-of-plane GNR structure, the electronic transport will be altered. We investigated the electronic transport properties of out-of-plane GNR intersections by computational method. The effect of inter-distance, width of GNR, external bias and stacking configurations is considered. The results demonstrate that inter-distance between GNRs affect the electronic transport properties of out-of-plane cross structure strongly. The larger the inter-distance becomes, the weaker the affection of out-of-plane cross connection will be, even under external bias. The out-of-plane GNR cross structures exhibit metallic behavior along the length direction of ZGNR when inter-distance is large enough. When inter-distance becomes smaller, some conductance dips appear in the transmission spectra because of the stronger interaction between two individual GNRs. Wider AGNR was found to bring stronger interaction into the system, and it will result in more transmission dips. Especially, conductance decreases appear near the charge neutral point when an external bias is added to the system along the length direction of ZGNR, for that the electron states distribution is changed by this bias. Moreover, the stacking configuration between the two GNRs was found to be crucial for the electronic transport under external bias, as it will affect the electronic transport properties strongly around the Charge neutral point. We believe our simulation results are helpful to the development of future graphene-based nanoelectronics.

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