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Low-energy band structures of armchair ribbon-graphene hybrid systems☆☆

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ABSTRACT

The electronic properties of armchair ribbon-graphene hybrid systems are studied within the $2p_z$ tight-binding model. The geometric structures of graphene nanoribbons, such as the width (N_y) and the period (R_y) of the ribbons, greatly determine the band structures. Furthermore, the stacking arrangement between graphene nanoribbons and monolayer graphene also plays an important role in low-energy states. Energy gaps caused by AA- and AB-stacking are dependent on N_ys and R_ys differently. These geometric structure effects can be well identified by the density of states.

1. Introduction

The few-layer graphenes, which had been realized through mechanical friction [1] and thermal decomposition [2], are well-known two-dimensional (2D) carbon-related materials. Moreover, monolayer and bilayer graphenes also display unconventional quantum Hall effects in transport properties [3,4]. Theoretical investigations of the electronic properties of the two systems have been made by using the tight-binding model [5–7] and density functional theory [8,9]. It is found that the energy dispersion near the Fermi level (E_F) is sensitive to the stacking arrangement as well as the layer number.

The quasi-one-dimensional (Q1D) graphene nanoribbons could be regarded as the graphene patterned into a narrow ribbon. Such fascinating materials could be produced by many physical treatments and chemical synthesis [10–12]. They are usually termed the zigzag and armchair graphene nanoribbons, corresponding to the zigzag and armchair shaped edges, respectively. The finite width and edge configuration make the electronic properties of the graphene nanoribbon different from those of graphene. For instance, in the armchair ribbon, the band structures would depend on the width due to the quantum confinement and have also been studied and reported theoretically [13–16].

2. Theory

The geometric structure of an armchair ribbon-graphene hybrid system is shown in Fig. 1(a). This hybrid system consists of the ribbons aligned periodically along the y-axis on the graphene. The width of ribbons is N_y and the period is R_y, and they denote the number of the dimer lines. The interlayer distance between ribbon and graphene is assumed to be $c = 3.35$ Å, which is the same as that of the graphite. The C-C bond length is $b = 1.42$ Å. The unit cell of this system has $(2N_y + 2R_y)$ carbon atoms, and its lengths along the x-axis and y-axis are $I_x = 3b$ and $I_y = \left(\sqrt{3}b/2\right)R_y$, respectively. The first Brillouin zone is defined by $-\pi/I_x \le k_x \le \pi/I_x$ and $-\pi/I_y \le k_y \le \pi/I_y$.

Considering the tight-binding model with the $2p_z$-orbitals of the carbon atoms, the Hamiltonian matrix in the electric field could be represented as

$$H = \begin{pmatrix} h_1 & h_{12} \\ h_{12}^* & h_2 \end{pmatrix}.$$

The block h_1 is a $2N_y \times 2N_y$ Hamiltonian matrix of the armchair graphene nanoribbon, whereas h_2 is a $2R_y \times 2R_y$ Hamiltonian matrix of the monolayer graphene. The elements of the h_1 and h_2 with the AB-stacking are given by

$$\left(h_{ij}\right)_1 = \begin{cases} \gamma_6 & \text{if } j = i, \quad i \text{ is odd;} \\ \gamma_0 e^{i\left(k_x b/2 + k_y\sqrt{3}b/2\right)} & \text{if } j = i+3, \quad i \text{ is odd;} \\ \gamma_0 e^{-i\left(k_x b/2 - k_y\sqrt{3}b/2\right)} & \text{if } j = i+1, \quad i \text{ is even;} \\ \gamma_0 e^{-ik_x b} & \text{if } j = i+1, \quad i \text{ is odd} \\ 0 & \text{others,} \end{cases} \tag{1}$$

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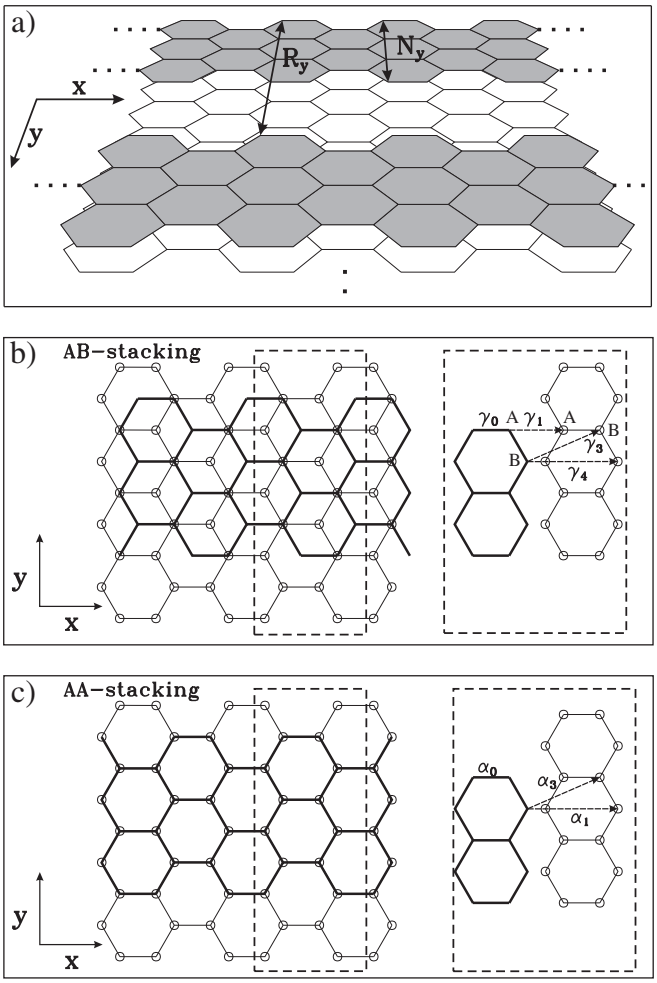

Fig. 1. (a) The geometric structure of an armchair ribbon-graphene hybrid system. N_y and R_y represent the ribbon width and period, respectively. (b) The ribbon is projected onto the graphene with the thick black lines in the AB-stacked hybrid system. γ_0 is the intralayer interaction and γ_is indicate the interlayer interactions. (c) same plot as (b), but shown for the AA-stacked hybrid system.

and

$$\left(h_{ij}\right)_2 = \begin{cases} \gamma_6 & \text{if } j=i, \quad i \text{ is even}, \ i<2N_y+4; \\ \gamma_0 e^{i\left(k_x b/2 + k_y\sqrt{3}b/2\right)} & \text{if } j=i+3, \quad i \text{ is odd}; \\ \gamma_0 e^{-i\left(k_x b/2 - k_y\sqrt{3}b/2\right)} & \text{if } j=i+1, \quad i \text{ is even}; \\ \gamma_0 e^{-ik_x b} & \text{if } j=i+1, \quad i \text{ is odd} \\ \gamma_0 e^{i\left(k_x b/2 - k_y\sqrt{3}b/2\right)} & \text{if } i=1, \ j=2R_y; \\ \gamma_0 e^{-i\left(k_x b/2 + k_y\sqrt{3}b/2\right)} & \text{if } i=2, \ j=2R_y-1; \\ 0 & \text{others}. \end{cases} \quad (2)$$

In this study, the armchair graphene nanoribbon and monolayer graphene are arranged according to Bernal (AB) stacking, as shown in Fig. 1(b). One atom (A atom) of the C-C bond is projected onto the A atom of the ribbon, and another (B atom) is projected onto the center of the hexagonal lattice. There exists a different value γ_6 between the on-site energies of A atom and B atom on the same layer due to the AB manner. In the ribbon (graphene), the A atom corresponds to the ith atom in which i equals odd integer (even integer).

In the h_{12}, the interactions of the $2p_z$ orbitals between the graphene nanoribbon and monolayer graphene with AB-stacking could be expressed by

$$\left(h_{ij}\right)_{12} = \begin{cases} \gamma_4 e^{-i\left(k_x b/2 + k_y\sqrt{3}b/2\right)} & \text{if } j=i, \quad i \text{ is odd}; \\ \gamma_4 e^{ik_x b} & \text{if } j=i+2, \quad i \text{ is odd}; \\ \gamma_4 e^{-i\left(k_x b/2 - k_y\sqrt{3}b/2\right)} & \text{if } j=i+4, \quad i \text{ is odd}; \\ \gamma_1 & \text{if } j=i+3, \quad i \text{ is odd} \\ \gamma_4 e^{-i\left(k_x b/2 + k_y\sqrt{3}b/2\right)} & \text{if } j=i, \quad i \text{ is even}; \\ \gamma_4 e^{-ik_x b} & \text{if } j=i+2, \quad i \text{ is even}; \\ \gamma_4 e^{-i\left(k_x b/2 - k_y\sqrt{3}b/2\right)} & \text{if } j=i+4, \quad i \text{ is even}; \\ \gamma_3 e^{i\left(k_x b/2 - k_y\sqrt{3}b/2\right)} & \text{if } j=i-1, \quad i \text{ is even}; \\ \gamma_3 e^{-ik_x b} & \text{if } j=i+1, \quad i \text{ is even}; \\ \gamma_3 e^{i\left(k_x b/2 + k_y\sqrt{3}b/2\right)} & \text{if } j=i+3, \quad i \text{ is even}; \\ 0 & \text{others}, \end{cases} \quad (3)$$

γ_0s and γ_is indicate the intralayer interactions and the interlayer interactions, respectively. That is, $\gamma_0 = 2.598$ eV, $\gamma_1 = 0.364$ eV, $\gamma_3 = 0.319$ eV, $\gamma_4 = 0.177$ eV, and $\gamma_6 = -0.026$ eV, corresponding to the values of the AB-stacked graphite [17].

Another arrangement in this hybrid system is the simple hexagonal (AA) stacking, as plotted in Fig. 1(c). In such a AA-stacking, all carbon atoms of the ribbon are projected directly onto those of the graphene. The corresponding intralayer and interlayer Hamiltonian elements can be expressed as follows:

$$\left(h_{ij}\right)_1 = \begin{cases} \alpha_0 e^{-ik_x b} & \text{if } j=i+1, \quad i \text{ is odd}; \\ \alpha_0 e^{i\left(k_x b/2 + k_y\sqrt{3}b/2\right)} & \text{if } j=i+3, \quad i \text{ is odd}; \\ \alpha_0 e^{-i\left(k_x b/2 - k_y\sqrt{3}b/2\right)} & \text{if } j=i+1, \quad i \text{ is even}; \\ 0 & \text{others}, \end{cases} \quad (4)$$

$$\left(h_{ij}\right)_2 = \begin{cases} \alpha_0 e^{-ik_x b} & \text{if } j=i+1, \ i \text{ is odd}; \\ \alpha_0 e^{i\left(k_x b/2 + k_y\sqrt{3}b/2\right)} & \text{if } j=i+3, \ i \text{ is odd}; \\ \alpha_0 e^{-i\left(k_x b/2 - k_y\sqrt{3}b/2\right)} & \text{if } j=i+1, \ i \text{ is even}; \\ \alpha_0 e^{i\left(k_x b/2 - k_y\sqrt{3}b/2\right)} & \text{if } i=1, j=2R_y; \\ \alpha_0 e^{-i\left(k_x b/2 + k_y\sqrt{3}b/2\right)} & \text{if } i=2, j=2R_y-1; \\ 0 & \text{others}, \end{cases} \quad (5)$$

and

$$\left(h_{ij}\right)_{12} = \begin{cases} \alpha_3 e^{i\left(k_x b/2 - k_y\sqrt{3}b/2\right)} & \text{if } j=i+3, \ i \text{ is odd}; \\ \alpha_3 e^{-i(k_x b} & \text{if } j=i+5, \ i \text{ is odd}; \\ \alpha_3 e^{i\left(k_x b/2 + k_y\sqrt{3}b/2\right)} & \text{if } j=i+7, \ i \text{ is odd}; \\ \alpha_1 & \text{if } j=i+4, \\ \alpha_3 e^{-i\left(k_x b/2 + k_y\sqrt{3}b/2\right)} & \text{if } j=i+1 \ i \text{ is even}; \\ \alpha_3 e^{i(k_x b} & \text{if } j=i+3, \ i \text{ is even}; \\ \alpha_3 e^{-i\left(k_x b/2 - k_y\sqrt{3}b/2\right)} & \text{if } j=i+5, \ i \text{ is even}; \\ 0 & \text{others}. \end{cases} \quad (6)$$

The hopping integrals α_0, α_1, and α_3 are taken from the simple hexagonal graphite in ref. [17]. By diagonalizing the Hamiltonian matrix, energy dispersion $E^{c,\,v}$ can be obtained, with the superscripts c and v representing the conduction π band and valence π band, respectively.

3. Results

Fig. 2(a) shows the band structures of the armchair ribbon-graphene hybrid system ($N_y = 18$, $R_y = 300$) along R-Y-Γ-X with $\Gamma(k_x = 0, k_y = 0)$, X$(\pi/\mathrm{I_x}, 0)$, Y$(0, \pi/\mathrm{I_y})$, and R$(\pi/\mathrm{I_x}, \pi/\mathrm{I_y})$. We only aim for the low-energy band structures for $k_x < 0.05$ 1/Å $\sim 0.068\,\pi/I_x$, and π/I_y is about one-sixth of 0.05 1/Å for $R_y = 300$. For the independent system, the low-energy band structures consist of the linear bands and