Electronic and transport properties of armchair graphene nanoribbons with defects

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Abstract—Density-functional theory (DFT) in combination with the nonequilibrium Green’s function formalism is performed to study the electronic and transport properties of armchair graphene nanoribbons with defects. The results show that the electronic and transport properties vary with different type of defects. The binding energy indicate that single-defect AGNRs are the most stable structure and line-defect AGNRs are the most unstable structure. The transmission spectra show that the defective AGNRs become disorder and the value decreases. The energy gap at the Fermi level become wider. These results would guide the experiments in real applications.

1. INTRODUCTION
Graphene, a two-dimensional structure of single-layer carbon atom, has shown excellent electrical, physical and mechanical properties[1-2]. Therefore, it’s known as a candidate for silicon. Graphene shows outstanding performance at sensors and solar cells[3-4]. However, graphene has no band gap, which can not be directly used in semiconductor devices [5-6]. Experimental and theoretical studies have shown that the electronic properties of graphene strongly depend on the shape and edge structure[7-8]. Graphene nanoribbons (GNRs) have two different edge structures: armchair and zigzag, which can display metallic or semiconductive property based on their different geometry configurations[9]. Theoretical calculations have indicated that the electronic and transport properties of GNRs can be modified by doping, defects, and external electrical field[10-12]. Defects will inevitably be introduced when graphene is patterned into nanoribbons. Therefore, the electronic and transport properties of armchair graphene nanoribbons (AGNRs) with different type of defects are studied systematically in this work.
2. METHOD AND MODELS

The AGNRs electron transport model consists of left and right electrode regions (indicated by black rectangles) and an intermediate scattering region, as displayed in Figure 1. The width of AGNRs is with \( N=6 \) carbon atoms. Each of the length of the electrode regions is 8.53Å and the length of the scattering region in each device is 38.39Å.

Density-functional theory (DFT) in combination with the nonequilibrium Green’s function formalism is carried out to study the electron transmission of AGNRs with defects in terms of H passivation. The Brillouin zone sampling is performed using \( 1*1*100 \) k-point sampling. The edges of AGNRs are passivated with H atoms. The AGNR with defects was optimized first. The local Density Approximations (LDA) and a 120 Ry cutoff were used in all the computations.

\[
T(E) = Tr\left[\Gamma_L(E)G^r(E)\Gamma_R(E)G^a(E)\right]
\]

where \( G^r(E) \) and \( G^a(E) \) represent the retarded and advanced Green functions of the scattering region, respectively. \( \Gamma_L(E) \) and \( \Gamma_R(E) \) are the imaginary parts of the self-energy of the left and right electrodes, respectively. They can be calculated by the following formula:

\[
\Gamma_{L,R}(E) = \delta(\sum_{L,R} - \sum_{L,R}^\dagger)
\]

where \( \sum_L \) and \( \sum_R \) are self-energy of left and right electrodes, respectively. They can be calculated by the following formula:

\[
\sum_L = H_{DL}g_LH_{DL}^\dagger \\
\sum_R = H_{DR}g_RH_{DR}^\dagger
\]

where \( H_{DL} \) and \( H_{DR} \) are the corresponding coupling matrix, respectively. \( g_L \) and \( g_R \) are the surface Green’s functions of left and right electrodes, respectively.

3. RESULTS AND DISCUSSIONS

To obtain stable geometry structures of the defected systems, we optimize the atomic structure of each defected configurations. The optimized configuration of AGNRs with different type of defects are displayed in Figure 2, single-defect AGNRs, two-defect AGNRs, three-defect AGNRs and line-defect AGNRs, respectively. The results show that after optimization, the bond lengths and bond angles near the defects have slight changes, as shown in Figure 2. After the defective AGNRs was relaxed, the formation energy of forming defects and the transmission spectra were calculated.

In order to investigate defect formation, the formation energy of forming the defects are calculated as
where $E_d$ and $E_p$ represent the total energy of defective AGNRs and perfect AGNRs, $n_i$ is the number of atoms, which have been added or removed to create the defect, $\mu_i$ is the chemical potential of atoms. The calculated $E_b$ for various structures is depicted in Figure 3. The value of $E_b$ can indicate that whether defects are easy to form. The results show that the single-defect structure are the most stable configuration, and the line-defect structure are the most unstable configuration. In the experiment, single-defect structures are more common than line-defect structures.

The transmission spectra $T(E)$ of different defective AGNRs are shown in Figure 4. The $T(E)$ of perfect AGNRs shows a sequence of steps and a energy gap appears at the Fermi level, which are characteristic features of armchair graphene nanoribbons. The energy gap at the Fermi level is around 1eV. With the increase of the absolute value of the electron energy, the intrinsic transmission coefficient increases by an integral multiple, indicating that the number of electron channels increases when the energy reaches a certain value. The $T(E)$ of all defective AGNRs decrease and become disorder. The transmission coefficient increases not by an integral multiple. All the defective transmission spectra has the similar shapes. It’s indicating that these kind of four type defects have the similar impact on the transmission properties. The energy gap of defective AGNRs are wider than the perfect AGNRs. This show that the introduction of defects reduce the transmission performance of AGNRs. The defective AGNRs have a small peak at the Fermi level. Figure 5 shows the density of states of different defective AGNRs. They have the same energy gap as in $T(E)$. The spots of the valleys in $T(E)$ are the peaks in the DOS.

Figure 2. AGNRs models with different type of defects. (a) Single-defect AGNRs. (b) Two-defect AGNRs. (c) Three-defect AGNRs. (d) Line-defect AGNRs.
Figure 3. The binding energy of AGNRs with different type of defects.

Figure 4. The transmission spectra of different defective AGNRs.

Figure 5. DOS of different defective AGNRs.
4. CONCLUSIONS
Graphene has attracted a lot of attentions in many exhibited potential applications, such as optoelectronics devices, sensors and FET. Although, it has shown excellent performance, known as potential candidate for the next electronic applications, it still has a long way from commercial applications. The huge issue is to open a band gap in graphene. A lot of efforts have been done to tailor graphene into dots or nanoribbons. However, defects are unavoidable to be introduced during fabrication. Therefore, it’s necessary to study the effect of defects on the electronic and transport properties of graphene nanoribbons.

In this paper, we investigated the electronic and transport properties of armchair graphene nanoribbons with defects using first-principles calculations. The results show that the electronic and transport properties vary with different type of defects. The binding energy indicate that single-defect AGNRs are the most stable structure and line-defect AGNRs are the most unstable structure. The transmission spectra show that the defective AGNRs become disorder and the value decreases. The energy gap at the Fermi level become wider. These results would guide the experiments in real applications.

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