Electronic conductance of a lengthy zigzag honeycomb nanotube including some surface-adsorbed molecules

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Abstract

The effect of the adsorption of environmental polyatomic molecules on the electronic transport properties of a lengthy zigzag honeycomb nanotube is investigated using the Green's function formalism within the tight-binding approach. We follow the theoretical approach in our previous paper, (Nadri *et al* 2019 *Chin. Phys*. B **28** 017202), which is done for a lengthy armchair honeycomb nanoribbon. Three types of adsorbed molecules are considered: di-, tri- and tetra-atomic ones which are located at a small part in the middle of the nanotube. The results show that in the presence of adsorbed molecules, the original band gap of the nanotube becomes wider and at some molecular concentrations the system converts to a n- or p-type semiconductor. In some molecular concentrations and configurations, a new energy gap is opened that can produce new physical aspects in nanotubes.

Keywords: nanotube, conductance, tight-binding, green's function

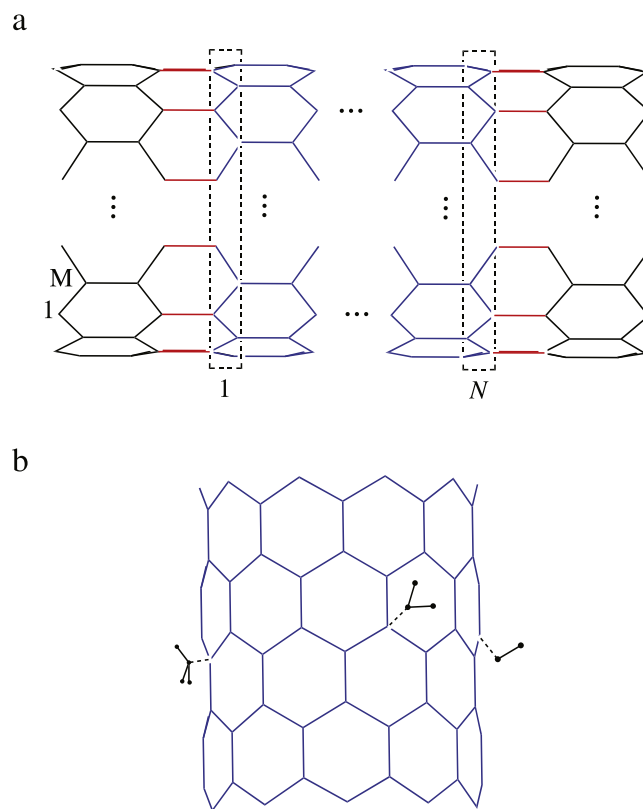(Some figures may appear in colour only in the online journal)

1. Introduction

Among all nanoscale materials, honeycomb structures, regarding their relatively low weight and unique mechanical properties, have found many applications in various industries. Compared to other atomic arrangements, the structures that are created by atoms in hexagonal formations, are stronger, more durable and flexible. Meanwhile, honeycomb nanotubes, single-walled ones, in particular, have attracted a great deal of interest in research due to their quasi one-dimensional architecture [1]. Since one-dimensional systems have remarkable differences from higher dimensional materials, physicists expect unique applications from them. Although single-walled carbon nanotubes are the first honeycomb nanostructures that were discovered [2] and the most popular ones, there are also different types of inorganic nanotubes with the hexagonal arrangements of atoms. Among those are BN, MoS_2 and GaS nanotubes [3]. The electronic properties of carbon nanotubes depend on their diameter and chirality. Based on these parameters, they can be conductors or semiconductors [4]. But since it is very difficult to produce

nanotubes with the same diameter and chirality and therefore identical properties, this feature is regarded as elimination in the use of these materials. On the other hand, boron nitride nanotubes are all semiconductors [5] and the band gaps of monolayers and single-walled nanotubes of IIB–VI semiconductors such as ZnO, CdO, ZnS and CdS, are independent of their diameter and chirality [6]. In many theoretical studies, honeycomb nanostructures are described with full network approximation and as disorder-free systems. But, in fact, even a perfect system is surrounded by an imperfect world. In one-dimensional systems, imperfections and disorders play significant roles in determining the physical properties. This is mainly because the charge carriers are confined to only one physical path and even a single center of scattering cannot be ignored. A nanotube interacts with its surrounding environment and depending on the interaction strength, the environmental effects can be as strong as the effect of defects and impurities inside the lattice network. Some environmental polyatomic molecules can connect to the atoms in the lattice surface and cause the change of electronic transport properties. Because of the curved surface of carbon nanotubes,

carbon atoms that are sp^2 hybridized, become susceptible to forming chemical bonds with other molecules through their inner or outer surfaces. Also, the curvature of the surface of them prevents the high compactness of carbon atoms. Therefore, carbon nanotubes may even be more sensitive than graphene sheets in the adsorption of environmental molecules [7–9]. Weak Van der Waals interactions of honeycomb surfaces even with simple molecules can result in significant changes in the electronic structure such as the band gap width and the concentration of charge carriers [10–12]. The band gap of some honeycomb nanotubes such as BN ones is so thin that it is suitable for nanoelectronic applications [13]. There are several ways to alter the band gap width of a nanoscale semiconductor including the effects of substrates [14], injection of impurities [15] or adsorption of particles [12, 16]. Unlike other methods, the physisorption of molecules on nanotube surfaces can be easily controlled while the damage caused by this method to the electronic structure of the nanotube can be very limited. So far, many studies have been performed in the adsorption of atoms and molecules on the surface of honeycomb nanostructures. Absorbed molecules can bind the surface through covalent or non-covalent bonds. For example, carboxyl (–COOH) and carbonyl (–COH) groups can covalently bond to graphene sheets [17] and nanotube surfaces [18] and change carbon atoms into sp^3 hybridized ones. In contrast, polycyclic aromatic hydrocarbons [19] bind graphene through non-covalent bonds. The connection of small gaseous molecules like H_2O and NO_2 on the graphene surface can cause p-type doping while NO, CO and NH_3 molecules can lead to n-type doping [20, 21]. The exposure of single-walled carbon nanotube to even small amounts of gaseous molecules like NH_3 and NO_2 results in a great variation of their electrical resistance, which is the basis of the operation of chemical sensors [12, 22, 23]. Moreover, the adsorption of several molecules with various sizes on graphite, graphene layers and carbon nanotubes is studied based on the molecular dynamics simulations [6]. *Ab initio* calculations show that the adsorption of hydrogen atoms and molecules on BC_2N nanotubes results in properties that are crucial for electronic applications. Depending on the hydrogen-absorbing sites, these nanotubes can reach donor or acceptor properties and they can be used as hydrogen storages [10]. Evaluation of the band gap changes of a BN nanotube, under the influence of non-covalent adsorption of an organic molecule with the effect of a transverse electric field, indicates that the band gap of the nanotube can be affected by poorly adsorption of the molecule [11]. This result is due to the presence of the electronic states of the molecule within the band gap of the adsorbate. The connected molecules can eliminate the rotational and translational symmetries of nanotubes. so sometimes the system becomes completely different from an ideal one. In fact, it is possible to modify the electronic properties of honeycomb nanotubes by absorbing the molecules. These results can open a new window in the modification of the electronic structure of nanomaterials to expand their applications in the nanoelectronics industry.

In this paper, we present a fast-calculating algorithm to investigate the electronic transport properties of a lengthy

Figure 1. (a) Schematic picture of an infinite perfect honeycomb nanotube with a disturbed region in the middle. The blue region (center wire) including N cells along the length and M atoms in each cell, is connected via red bonds (contacts) to black regions (left and right leads). (b) A zigzag nanotube with adsorbing some typical di-, tri- and tetra-atomic molecules.

zigzag honeycomb nanotube which has absorbed some typical polyatomic molecules via the tight-binding approach. In the symmetric cases, we drive analytical formulas for the transmission coefficient and density of states based on the Green's function technique. An understanding of the relation between the number and the type of adsorbed molecules on the system conductance is another aim of the paper.

In section 2, the theoretical model is introduced. Then, the numerical results are presented in section 3. Finally, section 4 gives a brief summary and concludes the results.

2. Theoretical model

In this section, we consider the conductance of a lengthy zigzag honeycomb nanotube including a different part at the center. According to figure 1(a), the center part (W) has N unit cells along the length, in which each unit cell has M (which is an even number) atomic sites. Two other parts (left (L) and right (R) leads) are assumed to be ideals with semi-infinite lengths. It is supposed that the center part can absorb some molecules in its external surface (see figure 1(b)). We assume the molecules are absorbed by the surface of nanotube through non-covalent bonds and only a single bond attaches the molecule to the nanotube. The model is based on the one

which is proposed in our previous work, [24], for a lengthy armchair honeycomb nanoribbon. The formalism for a zigzag nanotube coincides with it exactly, except for some differences that are mentioned as follows. First of all, two extra elements are in the Hamiltonian matrix of each unit cell in the leads and the center wire

$$(\mathbf{H}_{i,i})_{M,1} = (\mathbf{H}_{i,i})_{1,M} = \beta \qquad (1)$$

which corresponds to the closed boundary conditions (here β is hopping energy between nearest neighbors). Secondly, the unitary matrices used to transform the Hamiltonian of the ideal parts of the zigzag nanotube to the Hamiltonian of some equivalent polyacetylene-like (PA-like) chains with alternative β and $-2\beta\cos(2l\pi/M)$ hopping terms (l runs from 1 to $M/2$), read

$$(\mathbf{U}_1)_{m,n} = \frac{1}{\sqrt{M}}\exp(2\imath\pi mn \big/ M), \qquad (2)$$

$$\mathbf{U}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} -\mathbf{I} & \mathbf{I} \\ \mathbf{I} & \mathbf{I} \end{pmatrix}, \qquad (3)$$

where $\mathbf{I}$ is the identity matrix of size $M/2$ that is the number of obtained equivalent PA-like chains. Thirdly, the transformed matrices of the left (right) self-energy containing the self-energy functions of the center part in the presence of PA-like chains, read [25]

$$(\tilde{\Sigma}_{L(R)})_{m,n} = \tilde{\Sigma}_{L(R)}^{(n)}\delta_{m,n} = \tilde{\sigma}_{L(R)}^{(n-\frac{M}{2})}\delta_{m,n}$$
$$\text{for } \left(\frac{M}{2}+1\right) \leqslant n \leqslant M$$
$$\text{and otherwise } (\tilde{\Sigma}_{L(R)})_{m,n} = 0, \qquad (4)$$

where

$$\tilde{\sigma}_{L(R)}^{(l)} = \frac{\beta_{WL(R)}^2(\varepsilon - \varepsilon_{L(R)})}{(\varepsilon - \varepsilon_{L(R)})^2 - 4\beta^2\cos^2\frac{2l\pi}{M} - 2\beta^2|\cos\frac{2l\pi}{M}|(\xi_{L(R)}^{(l)} - \sqrt{\xi_{L(R)}^{(l)2} - 1})}, \qquad (5)$$

with

$$\xi_{L(R)}^{(l)} = \frac{(\varepsilon - \varepsilon_{L(R)})^2 - \beta^2\left(2\cos\frac{4l\pi}{M} + 3\right)}{4\beta^2|\cos\frac{2l\pi}{M}|}, \qquad (6)$$

where $l = n - M/2$, ε is the energy of the incoming electron and $\varepsilon_{L(R)}$ is atomic on-site energy in the left (right) leads. The electronic transmission coefficient of the system can be obtained using the following formula

$$T(\varepsilon) = \sum_{l=1}^{M/2} \frac{16\,\text{Im}\,\tilde{\Sigma}_L^{(l)}\,\text{Im}\,\tilde{\Sigma}_R^{(l)}\cos^2\frac{2\pi l}{M}}{\beta^2|\tilde{D}_N^{(l)}(\varepsilon, \tilde{\Sigma}_L^{(l)}, \tilde{\Sigma}_R^{(l)})|^2}, \qquad (7)$$

where

$$\beta^2\tilde{D}_N^{(l)}(\varepsilon, \tilde{\Sigma}_L^{(l)}, \tilde{\Sigma}_R^{(l)})$$
$$= \left((\varepsilon - \varepsilon_0)^2 - (\tilde{\Sigma}_L^{(l)} + \tilde{\Sigma}_R^{(l)})(\varepsilon - \varepsilon_0)\right.$$
$$\left. + \tilde{\Sigma}_L^{(l)}\tilde{\Sigma}_R^{(l)} - 4\beta^2\cos^2\frac{2\pi l}{M}\right)D_{N-1}^{(l)}(\varepsilon)$$
$$+ 2(\tilde{\Sigma}_L^{(l)}\tilde{\Sigma}_R^{(l)} - \beta^2)\left|\cos\frac{2\pi l}{M}\right|D_{N-3}^{(l)}(\varepsilon), \qquad (8)$$

where ε_0 is the on-site energy of atoms in the center part. Here, $D_p^{(l)} = \sin((p+1/2)\theta_l)\big/\sin(\theta_l/2)$ in which $p = N - 1$, $N - 3$ and $\theta_l = \cos^{-1}\left(((\varepsilon - \varepsilon_0)^2 - 2\beta^2\cos(4\pi l/M) - 3\beta^2)/4\beta^2\cos^2(2\pi l/M)\right)$. Finally, the density of states of ideal and non-ideal PA-like chain with on-site ε_0 and hopping β and $\beta_l'(=-2\beta\cos(2l\pi/M))$ energies, are

$$\text{DOS}^{(l)}(\varepsilon)$$
$$= \frac{2}{\pi}\frac{|\varepsilon - \varepsilon_0|}{\sqrt{4\beta^2\beta_l'^2 - ((\varepsilon - \varepsilon_0)^2 - \beta^2 - \beta_l'^2)^2}}; \quad \text{ideal} \quad (9)$$

and [26]

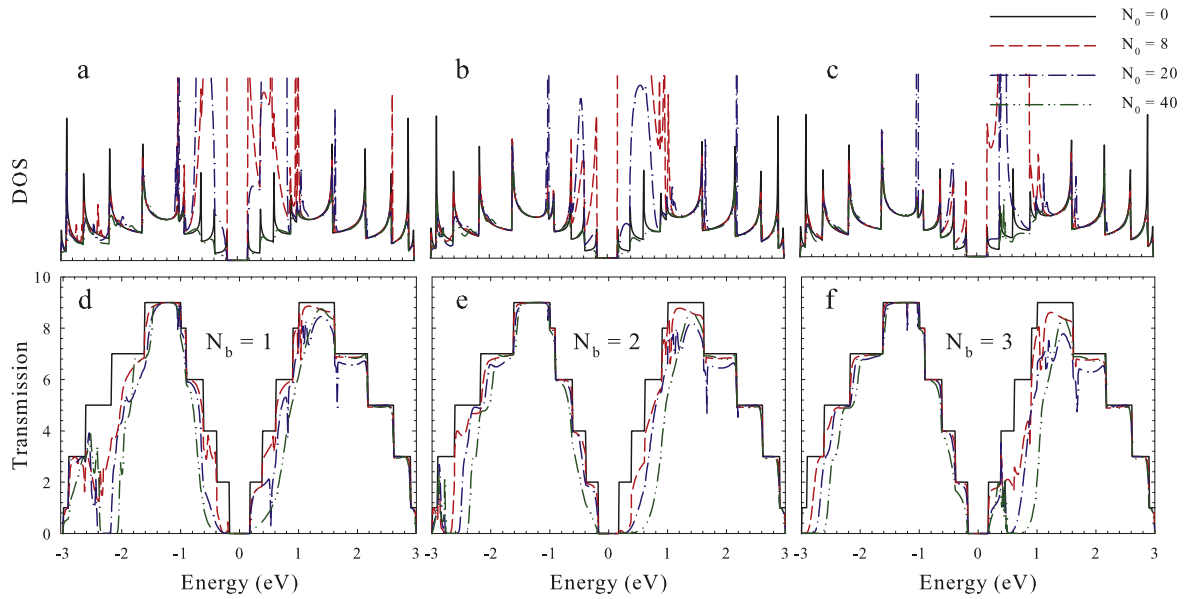$$\text{DOS}^{(l)}(\varepsilon) = -\frac{1}{\pi}\,\text{Im}\,\frac{\partial}{\partial\varepsilon'}\ln\tilde{D}_N^{(l)}(\varepsilon', \tilde{\Sigma}_L^{(l)}, \tilde{\Sigma}_R^{(l)})|_{\varepsilon'=\varepsilon};$$
$$\text{non-ideal} \qquad (10)$$

respectively. Therefore, we obtain DOS for an ideal zigzag nanotube as

$$\text{DOS}(\varepsilon) = \sum_{l=1}^{M/2}\text{DOS}^{(l)}(\varepsilon). \qquad (11)$$

Therefore, the formalism is provided for calculation of the electronic transport of a lengthy honeycomb nanotube including a different part at the middle. We mention here that when a polyatomic molecule is absorbed by an atom through physisorption in the center part of the nanotube, we could easily replace the on-site energy of that atom by a renormalized one [26, 27]. The formalism works for this situation after the mentioned change and the renormalized on-site will depend on the energy of the electron and tight-binding parameters of the added molecule. In the next section, we use the approach to compute the electronic transport properties of a lengthy honeycomb nanotube when in a part of it some typical polyatomic molecules are adsorbed. It is interesting to consider the effect of the number of atoms or branches in each molecule and the number of molecules themselves on the transport properties.

Figure 2. (a)–(c) and (d)–(f), respectively, show the density of states and transmission coefficient of a lengthy zigzag nanotube ($M = 20$) which has absorbed uniformly some typical di- ((a) and (d)), tri- ((b) and (e)) and tetra- ((c) and (f)) atomic molecules in a portion of its surface. Note that DOS belongs to the disturbed center region with $N = 4$. The values of all on-site and hopping energies of the clean system are set $\varepsilon_0 = 0$ and $\beta = 1$ eV, respectively. The other tight-binding parameters are taken as: $\varepsilon_M = 1.2$ eV, $\beta_b = 1$ eV and $\beta_c = 0.3$ eV.
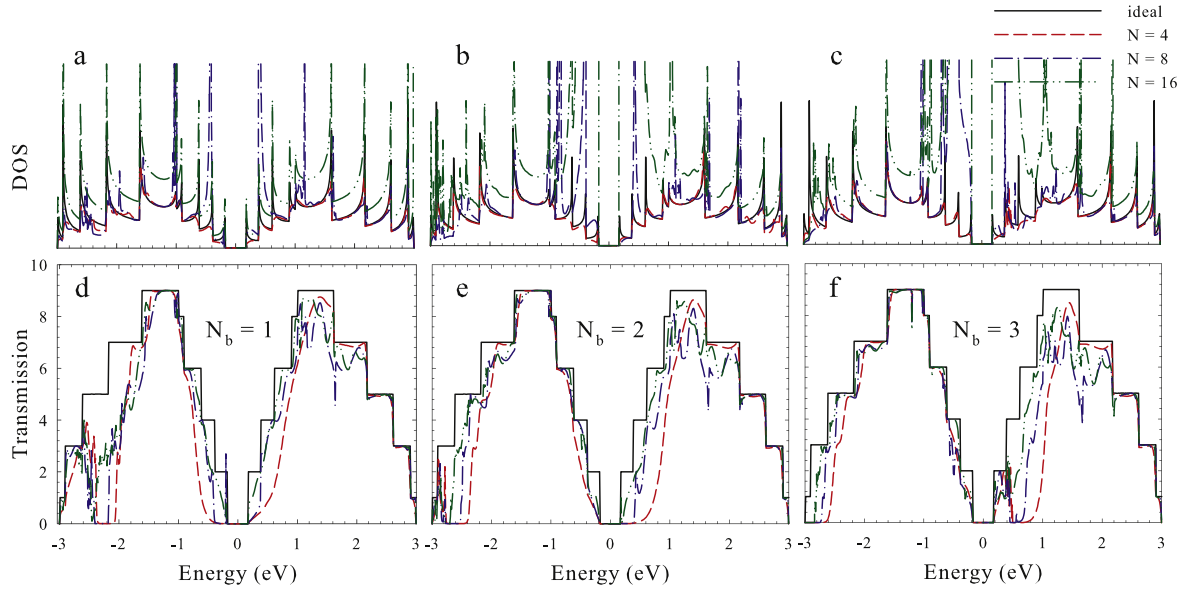
3. Results

Here, we examine the model for calculating the electronic transport properties of a lengthy typical honeycomb zigzag nanotube ($M = 20$) that has absorbed uniformly N_0 number of molecules in a small part of it. We suppose that the molecules are adsorbed in a way that they have the least effect on each other. We also neglect the particle-particle interactions and surface heterogeneity. Such simplifications have also been used in other studies [28]. To investigate the effect of the adsorption of different kinds of molecules on the nanotube surface, we focus on the parameters that have the most stronger effects on the conductance of the nanotube. The numerical results will be presented for di-, tri- and tetra-atomic molecules as shown in figure 1(b). We assume that all on-site and hopping energies in the ideal or clean nanotube are zero and one electron-volt, respectively. The renormalized on-site energy of the atom in nanotube which is connected to the absorbed molecule changes as

$$\varepsilon_0 \rightarrow \varepsilon_0 + \frac{(\varepsilon - \varepsilon_M)\beta_c^2}{(\varepsilon - \varepsilon_M)^2 - (N_b - 1)\beta_b^2}, \quad (12)$$

where ε_M is the on-site energy of each atom in the attached molecule. Also, β_b and β_c are the electron hopping energies between the neighbor atoms in the molecule and between the molecule and nanotube, respectively. Further, N_b is the number of bonds or branches in the molecule. First of all, we study the adsorption of different concentrations of molecules in certain locations of the nanotube's surface on the electronic transport properties. In this paper, we take the following typical values for tight-binding parameters in equation (12) as: $\varepsilon_M = 1.2$ eV, $\beta_b = 1$ eV and $\beta_c = 0.8$ eV.
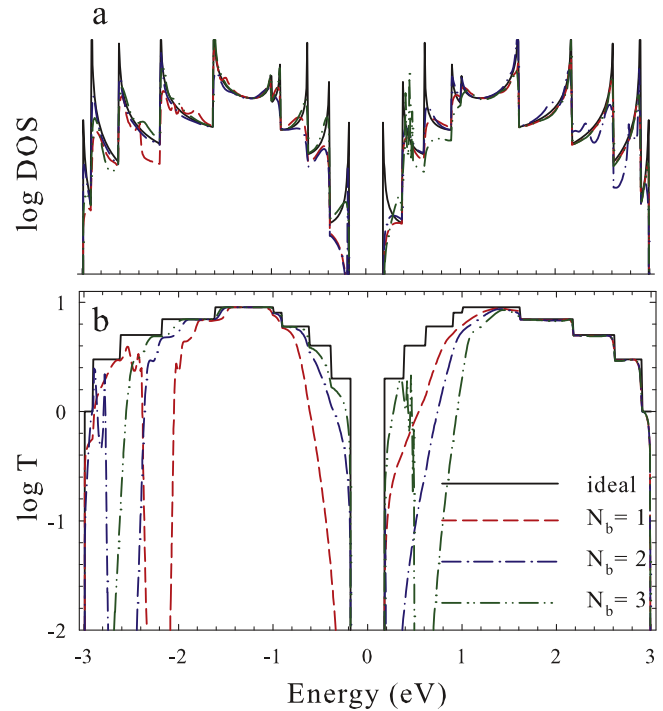
Figures 2(a)–(c) and (d)–(f) show the density of states of the middle part and the transmission coefficient of the system for some different values of N_0, respectively. Figures 2(a) and (d), (b) and (e) and (c) and (f) correspond to di-, tri- and tetra-atomic molecules, respectively. These molecules are supposed to be attached to a small part of the nanotube with length $N = 4$. This means that in each ring of the nanotube, there are $N_0/4$ added molecules. In this model, by using the mentioned values for the tight-binding parameters, the perfect nanotube is a semiconductor with a band gap of nearly 0.34 eV. Its transmission curve is a step function with a maximum value of 9 which is a result of the overlapping of $M/2 - 1 = 9$ conductance modes. The encounter of thin single-walled nanotubes with adsorbed molecules can effectively break their translational and rotational symmetry and deprive their electronic conductivity of the ideal form. According to the above-mentioned content in our model, it can be interpreted that the attached molecules change the on-site energies of corresponding connecting atoms according to equation (7) and consequently these affected atoms act as effective impurities. The curves of $T(\varepsilon)$ show that the band gap becomes wider in the presence of adsorbed molecules. When the number of absorbed molecules increases, in negative energies a valley appears in the conductance spectra that is dilated by increasing the molecular concentration. The experimental results [14] also indicate that the existence of molecules on the tube surface notably changes in the electrical conductance. In addition to molecular concentrations, the electronic conductivity of the nanotubes is highly sensitive to the structure of adsorbed molecules and the configuration of their attachments. Other researches also show that the electronic structure of honeycomb nanostructures such as the density of charge carriers and band gap, can be altered

Figure 3. (a)–(c) and (d)–(f), respectively, show the density of states and transmission coefficient of a lengthy zigzag nanotube with $M = 20$ which has absorbed uniformly a fixed number ($N_0 = 40$) of typical di- ((a) and (d)), tri- ((b) and (e)) and tetra- ((c) and (f)) atomic molecules in a small part it ($N = 4, 8, 16$). The values of all on-site and hopping energies are taken $\varepsilon_0 = 0$ and $\beta = 1$ eV, respectively, except tight-binding parameters related to the attached molecules which are chosen as $\varepsilon_M = 1.2$ eV, $\beta_b = 1$ eV and $\beta_c = 0.3$ eV.

with the adsorption of molecules [8, 20]. So, extensive manipulations of the electronic structure of these materials including n and p-doping are not only possible through molecular adsorption, but the effects may even be more severe than the edge effects and local defects [10–12]. Some experimental results [9] indicate that the existence of molecules on the tube surface notably changes in the electrical conductance.

In figures 3(a)–(c) to (d)–(f), we display the density of states of the middle part and transmission coefficient of the system for three different values of *N*, respectively. Figures 3(a) and (d), (b) and (e) and (c) and (f) correspond to di-, tri- and tetra-atomic molecules, respectively. Here, the number of adsorbed molecules is fixed: $N_0 = 40$. In the adsorption of all three kinds of molecules, for the smaller length of the center part, the width of the band gap located around zero energy further increases. For a uniform distribution of added molecules, when *N* is increased, the molecules are separated by greater distances leading to the reduction of molecular concentrations as well as the reduction of their effects on each other. As a result, for the more uniform distribution of the adsorption of molecules the less influence there is on the conductance of the nanotube. In the case of $N = 16$, there is a conduction valley in negative energies (for di- and tri-atomic cases) or in positive ones (for the tetra-atomic case) which is converted into a new energy gap by decreasing the length of the central part from $N = 16$ to $N = 4$. The location of this new energy gap depends highly on the type of molecules and the length of the central part. In all cases for $N = 8$ and 16, around the energy of $\varepsilon = 1.6$ eV, a sequential increasing and decreasing, is observed in the transmission spectra, which is known as the Fano phenomenon [29]. In this energy, the conductance of the ideal nanotube jumps into two stairs, which means the overlapping of conductance modes in the left and right of this stair, angle is different.

Figure 4. Logarithm of (a) density of states and (b) transmission coefficient of a lengthy zigzag nanotube with $M = 20$ in which the number of $N_0 = 40$ typical di-, tri- and tetra-atomic molecules are connected to the surface of its center wire with $N = 4$ width. The values of the on-site and hopping energies of the clean system are taken $\varepsilon_0 = 0$ and $\beta = 1$ eV, respectively and tight-binding parameters related to the attached molecules which are set as $\varepsilon_M = 1.2$ eV, $\beta_b = 1$ eV and $\beta_c = 0.3$ eV.

In order to compare the effect of the adsorption of different kinds of molecules on the nanotube conductivity, in figure 4 we plot $\log T$ and logDOS as the functions of energy for the case in

which the number of $N_0 = 40$ typical di-, tri- and tetra-atomic molecules are connected to the tube surface. Here, we fixed the length of the center wire as $N = 4$. The existence of all types of molecules makes the original band gap of the nanotube wider. The transmission curve corresponding to the case of the adsorption of tetra-atomic molecules has a band gap with the width of 0.3 eV out of the original nanotube band gap. This result is comparable to the experimental [30] and theoretical studies of the adsorption of NH_3 molecules on graphene sheets and nanoribbons [20, 31]. The figure also shows that by increasing the number of molecules, the band gap which had been created in negative energies shifts to lower energies.

4. Concluding remarks

The electronic conductance of a lengthy zigzag honeycomb nanotube which some environmental polyatomic molecules have attached on its surface is modeled by a fast calculating semi-analytical method based on the Green's function technique and the tight-binding approach. The formalism follows our previous work [24] which is for armchair honeycomb nanoribbons. In fact, the Hamiltonian of an ideal honeycomb nanotube is transformed into the Hamiltonian of some PA-like chains for periodic boundary conditions. Then, the effect of clean parts has been inserted into the transformed Green's function of the adsorbing region by the self-energy functions obtained by this transformed Hamiltonian. As an example, we numerically calculated the electronic transmission coefficient and density of states of a zigzag honeycomb nanotube with some typical di-, tri- and tetra-atomic molecules which are added on a small part. The results show that the adsorption of molecules generally reduces the electronic conductance and changes the original band gap around zero energy. This effect is high enough that by increasing the number of molecules, it can lead to a semiconductor-insulator transition. At some molecular concentrations and configurations, a new energy gap appears that can cue new electronic properties.

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