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A Computational Study of Quantum Transport Properties of Hydrogen Passivated Graphene Monoxide: NDR and Rectification

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Abstract

We computed the electronic transport properties of a structure analogue to graphene monoxide using combining non-equilibrium Green's function (NEGF) and density functional theory (DFT) methods. These properties were transmission spectrum and current-bias voltage characteristics, along with density of states (DOS) and projected density of states (PDOS) of the electrodes and central molecules. We found that the computed current values in considered bias potentials had the rectification behavior and included a negative differential resistance (NDR) region. We interpreted these properties using the relative localization and delocalization of molecular projected self-consistent Hamiltonian (MPSH) orbitals.

Keywords: graphene monoxide; negative differential resistance; molecular projected self-consistent Hamiltonian; non-equilibrium Green's function; density of states.

1. Introduction

The study of electron transport properties of molecules and nano structures, as the electronic components used to produce low-dimension circuits, has been taken in to consideration in the past decade [1-4]. Recently, some researchers have reported interesting properties of such molecules and nano structures like rectification[5,6] Negative Differential Resistance (NDR)[7,8] and switching effect[9,10].

Historically, molecular rectifiers were the first molecular electronic components proposed by Aviram and Ratner in 1974[11]. In their approaches, an organic molecule with donor and acceptor parts was separated by a sigma-bridge, showing rectification and acting as a p-n junction. Afterwards, the experimental results of a research carried out by Metzger and co-workers[12] showed the rectifying behavior in Metal-Insulator-Metal contact. Further studies revealed that the functionalized molecules with donor-acceptor groups [13], structures with asymmetrical configurations [14], or asymmetrical contact to the electrodes[15] exhibited rectification.

Decreasing current with increasing bias voltage is another important phenomenon in nano electronic systems and is known as NDR. This behavior is the basis of different electronic devices such as resonant tunneling diodes [16], and switches [17], which are important components in memories and molecular electronic logic circuits.

In recent years, a lot of experimental and theoretical works on NDR phenomenon have been performed [18,19]. In this regard, some structures such as DNA [20], nanotubes[21], and organic molecules[22] displaying NDR behavior have been introduced. The NDR behavior has been interpreted using mechanisms based on charge transfer[23], charge storage[24] and the possibility of polaron formation on the molecular wire[25].

Two-dimensional nano structures such as graphene and derivatives containing hetero atoms like oxygen have been investigated to a large extent [26-28]. One of newly synthesized graphene derivatives containing oxygen with interesting electronic properties, such as direct band gap of about 0.9 eV[29], is graphene monoxide (GMO). In recent years, various researchers have reported some theoretical and experimental studies on GMO. Refs 30-34 include computational calculation of structural, optical, mechanical and heat transport properties of GMO and some variants of it[30-34]. Despite many modern applications of the electronic transport properties, these properties of GMO have not been studied yet. However, in order to provide reliable computational results and to continue the previous publications of this team[35,36], the electronic transport properties of GMO were computed by density functional theory (DFT) combined with the non-equilibrium Green's function (NEGF) method. Electronic transport properties computed here included transmission spectrum, current-bias voltage ($I-V_b$) curve and rectification ratio. These computations were carried out at the V_b ranging from -2.5 V up to 2.5 V divided by 0.1 V intervals. The $I-V_b$ curve and its variations were discussed in terms of transmission spectrum, density of states (DOS) and molecular projected self-consistent Hamiltonian (MPSH)

of the considered system. The results showed that the considered system had a significant rectification ratio and NDR regions in $I-V_b$ curve.

2. Models and methods

On the basis of recent studies reported by other researchers[37], a polycyclic structure was taken and computationally oxidized for giving a GMO homologue structure. In order to study the quantum transport properties arising from structural asymmetry, the considered symmetrical GMO homologue was functionalized by an electron donor group and an electron acceptor group. The effect of asymmetry on the quantum transport properties had been studied by several researchers[38,39].

The functionalization was carried out by the substitution of two hydrogens by an amino group and a nitro group as donor and acceptor segments, respectively. Then the structure was optimized using density functional theory (DFT). The considered structure was laid between two aluminum atomic chain electrodes as shown in Fig.1.

All density functional theory computations were carried out using conjugated gradient algorithm implemented in Spanish Initiative for Electronic Simulations with Thousands of Atoms (SIESTA) software package[40]. In all our DFT calculations, we used general gradient approximations (GGA) exchange-correlation functional parameterized by [41]. Also, Troullier-Martines pseudo-potential[42] was used for core electrons and double zeta plus polarized (DZP) basis sets for valence electrons. **We have adapted 150 Ry plane wave cutoff.** In order to compute the electronic transport properties, Non-Equilibrium Green's function (NEGF) techniques combined with DFT method were used through TranSiesta code[43]. In the implemented method, the

considered systems were separated to three regions including semi-infinite left and right electrodes and a contact region. The contact region, C, had a functionalized central molecule along with four atoms of the electrodes in each side.

The distances between Al atoms in the electrodes were chosen to be 2.30 Å, according to Adam J. Simbeck *et.al* [44]. There was a band gap below the Fermi energy in the band structure of aluminum atomic chain computed in this ref. The existence of such band gaps in the band structure could play an essential role in electronic transport properties.

The distances between electrodes and molecules in the left and right sides were 1.84 Å and 1.83 Å respectively, as obtained by scanning the energy with respect to electrode-molecule distance. The electrodes were attached to the molecule via its carbon atoms according to Fig.1.

In the implemented TranSiesta method[43], Green's function matrix obtained from the following DFT Hamiltonian was calculated for the finite part of system represented by L-C-R in Fig.1:

$$H = \begin{bmatrix} H_L + \Sigma_L & V_L & 0 \\ V_L^\dagger & H_C & V_R \\ 0 & V_R^\dagger & H_L + \Sigma_R \end{bmatrix} \quad (1)$$

where H_L , H_R and H_C are the Hamiltonian matrices in L, R and C regions; Σ_L and Σ_R are self-energies for L and R regions; and V_L (V_R) is the interaction between C and L (R).

The self-energy terms express the coupling between L (R) region to the remaining part of the semi-infinite electrodes. Determination of V_L , V_R and H_C was done by the self-

consistent procedure using non-equilibrium electron density without any information about outside L-C-R region.

The Landauer–Buttiker formalism[45] was used to calculate the current, I , in the contact region:

$$I(V) = \frac{2e}{h} \int_{-\infty}^{+\infty} d\varepsilon T(\varepsilon, V_b) [n_f(\varepsilon - \mu_L) - n_f(\varepsilon - \mu_R)] \quad (2)$$

n_f and $\mu_{L(R)}$ are Fermi occupation function and the electrochemical potential of left (right) electrodes, respectively. μ_L and μ_R are given by the following equations in terms of Fermi energy and bias potential;

$$\mu_L = E_f + \frac{eV_b}{2} \quad (3)$$

$$\mu_R = E_f - \frac{eV_b}{2} \quad (4)$$

$$\mu_L - \mu_R = eV_b \quad (5)$$

And $T(\varepsilon, V_b)$ is the transmission function between the electrodes at energy ε and under the bias potential V_b :

$$T(\varepsilon, V_b) = \text{Tr} [\Gamma(\varepsilon) G^\dagger \Gamma_R(\varepsilon) G(\varepsilon)] \quad (6)$$

where $\Gamma_{L(R)}(\varepsilon)$ is the contact broadening function obtained from the self-energy describing the coupling between L (R) and C regions.

In this research work, the computations on the electrodes were performed in the periodic boundary conditions with $1 \times 1 \times 100$ k-point sampling in Brillouin zone (BZ), according to Monkhorst-Pack approaches[46]. The unit cell of electrodes included four aluminum atoms, while transport calculations were done only at Γ point. On the basis of a recently published article, the I - V_b characteristics were computed in a bias voltage ranging from -2.5 up to +2.5 V and divided by 0.1 V step sizes.

3. Results and discussion

The current-bias voltage characteristic of the studied system is presented in Fig. 2(a). This figure shows that the system acted differently in positive and negative bias values. This arose from the asymmetrical structure of the considered system. A close examination of this figure showed that the current was nearly constant without any special features in the negative values of V_b . This behavior was continued at the positive biases up to 1.2 V. However, two jumps in the current curve were observed at $V_b=0.1$ and 1.2 V, and a sharp fall occurred beyond 1.6 V. This sharp fall in the current led to Negative Differential Resistance (NDR) in the current-bias curve. Fig. 2(b) presents rectification ratio, RR, which is defined as the ratio of the current in the positive bias to the negative ones ($RR=I_+/I_-$). This figure also shows that RR started from the values near 5 until reaching its maximum value (app. 21) at the bias value of 1.4 V. The values of rectification ratio underwent considerable decreases beyond 1.6 V bias voltage.

According to equation 6, the current would be computed from transmission function, $T(E,V)$, in the corresponding bias window (BW). Transmission probability in

a certain energy level depends on two factors: 1) existence of energy states in the same energies in DOS spectrum of electrodes and molecule; and 2) spatial distribution of molecular orbitals in these energies. General computational results[47,48] show that the transmission probability is relatively small when the frontier molecular orbitals are localized.

The transmission spectrum in zero bias voltage for the considered system is presented in Fig. 3(a). This figure shows that there was a small peak around the Fermi energy level which was inside BW at the low bias voltages. To understand $T(E,V)$ behavior, we considered the density of states (DOS) of electrodes and the projected density of states (PDOS) of molecule shown in Fig. 3(b).

This figure reveals that there was a gap in the energy interval of -0.4 eV up to -1.2 eV for both DOS electrodes and PDOS of molecules. As can be seen in these figures, for DOS electrodes, PDOS molecules and transmission spectra, the transmission coefficient in this gap region was zero because there was no state to create transmission channel.

Fig. 4(a)-(c) represents the molecular projected self-consistent Hamiltonian, MPSH, for HOMO-1, HOMO and LUMOs shown, HOMO was delocalized over the molecule; however, HOMO-1 and LUMO were localized over donor and acceptor parts, respectively. So, despite the existence of energy states, the HOMO-1 and LUMO states did not have any contribution in the transmission spectrum. The MPSH eigenvalues can be seen in Fig. 3(b) on the molecular PDOS curve.

In TranSIESTA method, the chemical potentials of the left (right) leads were shifted by the value of $V_b/2$ ($-V_b/2$), according to equations (3) and (4). This potential

caused a shift in the energy states of the electrodes with respect to each other. Fig. 5(a)-(d) shows DOS of electrodes, PDOS of molecule and transmission spectrum in the bias values of -1.4, +1.4, +1.6 and +2.0 V. The results showed that in the negative bias voltages, the numerical value of transmission was small and consequently, the current was smooth and small. On the other hand, in the positive bias voltages, the transmission peak near the Fermi level lied inside the BW and the current values could get a larger magnitude. So, the considered device would be at “off” state under negative biases and in positive biases, would fall in “on” state. Therefore, the studied device could be used as a rectifier. However, enhancing the positive bias voltages decreased the overlap of gap regions in DOS electrodes spectrum. This overlap was vanished in the bias voltage of 0.8 V. This caused the formation of a transmission peak in about -0.8 eV to be outside bias window. Therefore, this small peak did not contribute in the current values. However, this peak was perched in the bias window at the bias value of 1.3 V, and the current began to increase with a high slope up to a current value of 508.41 nA at the bias of 1.6 V. Fig. 5(c) also shows that at the bias of 1.6 V, the peak area completely lied in the BW region. Then, at the bias range of 1.6 V to 2.0 V, the height of transmission peak and so, the integrating area and the current would be reduced. This led to an NDR region in $I-V_b$ curve. The emergence of an NDR in $I-V_b$ curves suggested that we could use the considered device as a nano-switch.

In order to interpret the computed current's behavior at the NDR region and the observed trend in $I-V_b$ characteristics, the MPSH orbitals were considered. Figures 6(a) and 6(b) present MPSH orbitals of the considered device at the energy values of -0.574 eV and -0.596 eV for the bias values of 1.6 and 2.0 V, respectively. These bias

potentials and energies correspond to the limits of NDR region and the transmission peak of figure 5, respectively. It has been verified by computational methods^{46,47} that in some cases, there are more localized MPSH orbitals, less transport channels and consequently, lower electrical current. The results of these figures showed that in the bias value of 2.0 V, the MPSH orbitals were localized on the donor-bound part of the device. This localization of MPSH orbitals led to a reduction in transmission and consequently, in the current. Figure 6(b) shows that at a lower bias potential, say 1.6 V, the MPSH orbital is totally delocalized and spread out over the device. This delocalization of MPSH orbitals leads to the creation of the transmission channels and therefore, transmission probability rises up to the higher values.

4. Conclusions

The electronic transport properties of a nano-structure analogue of graphene monoxide were computed using NEGF-DFT method. The transmission spectrum and electrical current were evaluated at a bias voltage ranging from -2.5 V to +2.5 V and divided by 0.1 V sized intervals. The obtained results showed relatively small current values, or “off” state of the device in the negative bias voltages, while in the positive bias values, current rose up to a relatively larger magnitude or the device fell to the “on” state. These results implied that the studied structure showed a rectifying behavior. Also, there was a NDR region in the bias range of 1.6-2.0 V. The NDR behavior was verified by overlapping energy gaps in DOS spectrum of electrodes, and also interpreted using the relative localization and delocalization of MPSH orbitals in the considered energies.

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Figure captions

Fig. 1 The two-probe model of our considered system, functionalized molecule added by four Aluminium atoms in each side (C) along with semi-infinite left (L) and right (R) Aluminium electrodes.

Fig. 2. (a) Two probe $I-V_b$ curves with the voltage applied to lead left and right. Negative V_b and low positive V_b lead to a negligible current. At higher positive V_b (above 1.3 V), we have nonlinear $I-V_b$ curves. (b) Rectification ratio curve.

Fig. 3. (a) Zero bias transmission spectra of considered system (b) PDOS of the central molecule and LDOS (DOS of the left electrode) at zero bias; small blue triangles represent the MPSH eigenvalues for the HOMO-1, HOMO and LUMO.

Fig. 4. MPSH for (a) HOMO-1 (b) HOMO and (c) LUMO at zero bias

Fig. 5. The transmission spectrum and DOS for the considered system under (a) $V_b = -1.4$ V, (b) $V_b = +1.4$ V, (c) $V_b = +1.6$ V and (d) $V_b = +2.0$ V. The red lines indicate the bias window; PDOS refers to the projected DOS of the central molecule, LDOS and RDOS refer to the DOS of the left and right electrodes, respectively.

Fig. 6. Molecular projected self-consistent Hamiltonian, MPSH for (a) $V_b = 1.6$ V in -0.574 eV and (b) $V_b = 2.0$ V in -0.596 eV.

Fig. 1.

For Review Only

Fig. 2.

Fig. 3.

Fig. 4.

Fig. 5.

Fig. 6.