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Temperature dependence of I-V characteristics of C_{60} molecule

S A Ketabi[1], E Mozafari[2] and N Shahtahmasebi[2]

1. School of Physics, Damghan University of Basic Sciences, Damghan, Iran
2. Department of Physics and Center for Nanotechnology Research, Ferdowsi University of Mashhad, Mashhad, Iran
E-mail: saketabi@dubs.ac.ir

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Abstract

Making use of a generalized Green's function technique and Landauer formalism, the temperature depended current-voltage (I-V) characteristics of C_{60} molecule, sandwiched between two metallic electrodes are numerically investigated. In addition, the influence of the electron-phonon coupling strength on the electronic properties of the molecule is studied. The I-V characteristics of the molecule are determined in two temperature limits, T=3K and T=300K. Our results indicate that the molecule primarily acts as a semiconductor in lower temperatures but moves toward becoming an ohmic-like conductor when the temperature increased to the higher magnitudes.

Keywords: current-voltage characteristic, C_{60} molecule, electron-phonon coupling, Landauer formalism

1. Introduction

The recent advent of nano electro-mechanical systems (NEMS) have attracted tremendous interests, both for practical applications and also as a fundamental theoretical area of research [1-7]. Despite the impressive progress achieved, there are still many important issues of physical properties that need to be resolved before NEMS become a viable technology. At a truly molecular scale, how then does the coupling of the different functional units affect on the electron transport? What is the role of the electrode/molecule interface? Which factors critically influence the current flow? All these questions need a thorough investigation in order to gain a fundamental understanding of the operation of the NEMS devices.

In this paper, we numerically investigate the influence of the electron-phonon coupling strength on the electronic properties of C_{60} molecule in metal/C_{60}/metal system. In addition, the role of the increase of the temperature leading the molecule toward the ohmic-like behavior is studied. The choice is motivated by the recent fabrication of a C_{60} amplifier [1]. The fullerene C_{60} is a soccer-ball-like structure consisting of 12 pentagons surrounded by 20 hexagons which make an almost spherical shape (figure 1). This all-carbon molecule can be produced by evaporation of graphite and can be isolated as soluble well-defined crystals where the C_{60} molecules solidify in a nearly closed packed face-centered-cubic (fcc) lattice at room temperature and undergo a structural transformation to a simple cubic (sc) with orientational order at a lower temperature [8].

In order to make progress in the understanding of complex phenomena, we need to describe the complexity of the one-body problem in terms of a simple model which captures the significant features of the electronic structure and conductance properties of the molecule. In this work, we numerically study the extent to which the realistic features of the conductance of the molecule may be understood within the nearest-neighbor tight-binding Hamiltonian. The model and description of the computational methods for investigating the conductance properties of the model structure are introduced in section 2. The results and discussion are presented in section 3, followed by a summary and a conclusion in section 4.

2. Computational scheme

The most commonly used computational schemes for calculating the (coherent) conductance g are the Landauer theory [9] and the Green's function formalism [10,11]. The conductance g is simply proportional to the transmission coefficient, $T(E)$, for injected electrons at the Fermi energy;

$$g = \frac{2e^2}{h} T(E), \qquad (1)$$

where the transmission function *T(E)* represents the

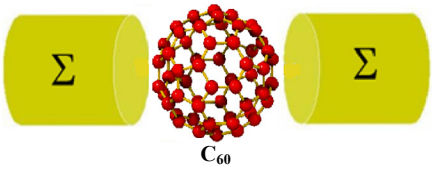

Figure 1. (Colour online) This plot shows a schematic representation of the metal/C_{60}/metal structure. As explained in the text, the left (right) contact is considered as a semi-infinite metallic electrode, described by an effective self-energy Σ.

transmission probability between the metallic leads for an electron with energy E. The metallic leads are simply modeled as one-dimensional tight-binding Hamiltonian and the metal/molecule coupling is described by the elements of the hopping matrix, $t_L(=t_R)=t_c$ which coupled with an arbitrary numbers of atomic orbitals of the C_{60} molecule to the metallic contacts on the left (right) side of the molecule.

The Hamiltonian of the molecule, H_M is described within the tight-binding approximation. It only treats the π-electron system with a basis of $2p_z$ atomic orbitals. The interactions are restricted to the electron hopping between nearest neighbors. Thus;

$$H_M = -\sum_{l',l} t_{l',l}(c_{l'}^{+}c_l + h.c.)\,, \qquad (2)$$

where the values of the hopping terms depend on the C-C bond lengths. One may consider the following simple relation between the hopping integrals and the bond lengths $R_{l',l}$ [12];

$$t_{l',l} = t_0 e^{-\alpha(R_{l',l}-R_0)}\,, \qquad (3)$$

α=0.8 Å^{-1}, $R_0 = 1.4$ Å and $t_0 = -2.5$ eV are the electron-phonon coupling constant, the reference bond length and the hopping integral, respectively. These parameters give a good fit to the experimental band width and band gap. The values of $R_{l',l}$ are obtained using the atomic coordinates achieved from fullerene library in Gaussian03 and the following simple relation;

$$R_{l',l} = \sqrt{(x_{l'}-x_l)^2+(y_{l'}-y_l)^2+(z_{l'}-z_l)^2}\,. \qquad (4)$$

Considering the effects of the left (L) and right (R) metallic contacts on the C_{60} molecule as the complex self-energy potentials $\Sigma_{L,R}(E)$, the Green's function of the system given as;

$$G(E) = [E - H_M - \Sigma_L - \Sigma_R]^{-1}\,. \qquad (5)$$

Using Dyson equation, the self-energy $\Sigma_L(=\Sigma_R)=\Sigma(E)$ may be carried out as [13];

$$\Sigma(E) = \frac{t_c^2}{E-\varepsilon_m-\Gamma}\,, \qquad (6)$$

where $\Gamma(E)$ is the self-energy correction of the metallic contacts to the ending-sites attached to the C_{60} molecule, and has the following expression [14];

$$\Gamma(E) = \left(\frac{E-\varepsilon_m}{2}\right) - i\left[t_m^2 - \left(\frac{E-\varepsilon_m}{2}\right)^2\right]^{1/2}\,. \qquad (7)$$

Here $\varepsilon_m = 0$ and $t_m = 1$eV are the onsite energy and the nearest-neighbor hopping integral of the metallic contacts, respectively.

The transmission coefficient can be calculated from the knowledge of the molecular energy levels, the nature and the geometry of the contacts. To connect the Green' function with the transmission coefficient between reservoirs we consider a linear transport between them. Using the Fisher-Lee formalism [15] the transmission coefficient may be expressed as;

$$T(E) = \left|G_{LR}(E)\right|^2 \Delta_L(E+eV)\Delta_R(E)\,, \qquad (8)$$

where $G_{LR}(E)$ is the matrix element of $G(E) = \left(E - H_{eff}\right)^{-1}$ between the left and right sides of C_{60} molecule coupled to the left and right contacts, respectively. H_{eff} is the Hamiltonian of the metal/C_{60}/metal system and making use of the Löwdin's matrix partition technique [16], we may write H_{eff} as follow;

$$H_{eff} = -\Sigma_L\left|L\right\rangle\left\langle L\right| + H_m - \Sigma_R\left|R\right\rangle\left\langle R\right|\,, \qquad (9)$$

where $\left|L\right\rangle$ and $\left|R\right\rangle$ denote the electron states on the left and right sides of the molecule connected to the left and right metallic electrodes, respectively.

To simplify the calculations, $\Delta_L(=\Delta_R)=\Delta$ is considered, where $\Delta = -\mathrm{Im}\{\Sigma\}$ is the chemisorption's coupling at the electrode/molecule interface. Thus, the effect of the metallic electrodes may be lumped into the energy of the molecular sites that coupled to the electrodes.

3. Results and discussion

In this section, at first we will study the electron-phonon coupling strength, α on the conductance of metal/C_{60}/metal system. Figures 2 and 3 illustrate, at room temperature (T=300K), the electronic density of states (DOS) and the logarithm of the transmission function of the system, respectively. The increase of α induces the decrease of the conductance of the system, as cleared. In fact, increasing of the electron-phonon coupling strength, the electronic states vanished in the energy gap give rise to lower transmittance through the molecule, as clearly shown in figures 2 and 3 for DOS and the electronic transmission through the molecule.

In order to calculate the current through metal/C_{60}/metal structure, we consider the standard transport formalism

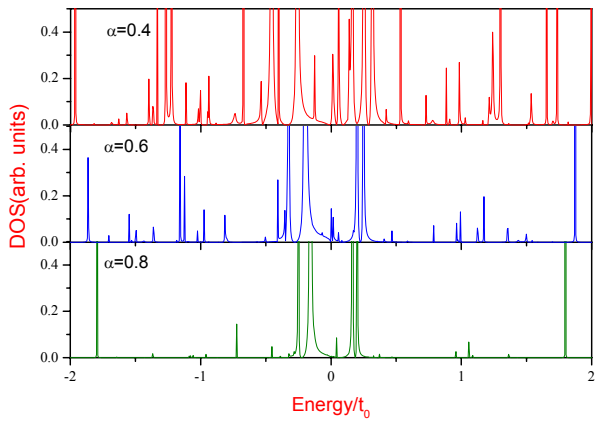

Figure 2. (Colour online) Electronic density of states (DOS) versus the dimensionless parameter $Energy/t_0$ at room temperature for the metal/C_{60}/metal system calculated for different values of α, the electron-phonon coupling constant and the molecule/electrode coupling strength $t_c = -0.3\,\mathrm{eV}$.

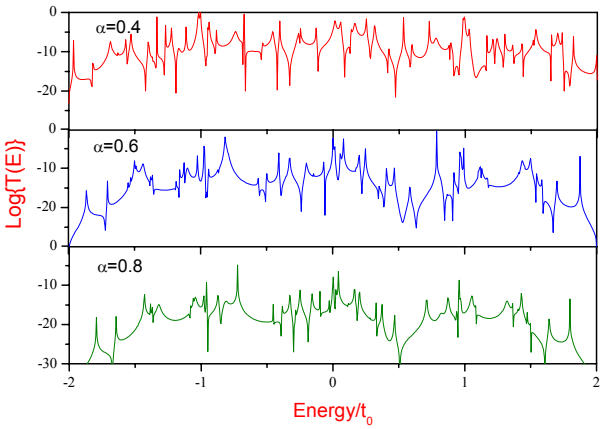

Figure 3. (Colour online) The logarithm of the transmission coefficient versus the dimensionless parameter $Energy/t_0$ at room temperature for the metal/C_{60}/metal system calculated for different values of α, the electron-phonon coupling constant and the molecule/electrode coupling strength $t_c = -0.3\,\mathrm{eV}$.

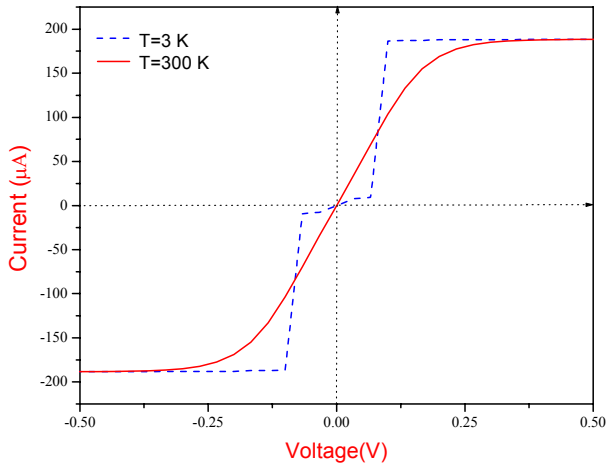

Figure 4. (Colour online) The current-voltage characteristics of C_{60} molecule at lower temperature (T=3 K, step-like dashed curve) and at room temperature (T=300 K, smoothed solid curve) in the metal/C_{60}/metal system. Using the model parameters as mentioned in the text, $t_c = -0.3\,\mathrm{eV}$, α=0.8 Å^{-1} and $t_0 = -2.5\,\mathrm{eV}$ are set.

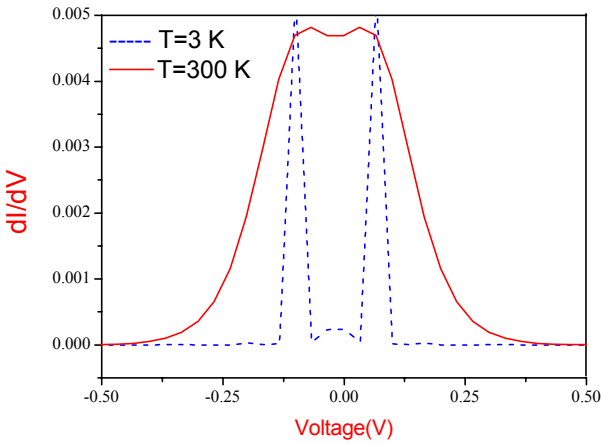

Figure 5. (Colour online) The differential conductance versus the applied bias between C_{60} molecule ends at lower temperature (T=3 K, dashed curve) and at room temperature (T=300 K, solid curve) in the metal/C_{60}/metal system. The model parameters are chosen according to figure 4.

of electric current under an applied potential bias of V [17,18];

$$I = \frac{2e}{h}\int_{-\infty}^{+\infty} dE\,T(E)W(E-E_f;\mathrm{eV}), \qquad (10)$$

where $T(E)$ denotes the electron transmission coefficient for the molecule in the metal/C_{60}/metal structure and E_f is the Fermi energy of the metallic electrodes;

$$W(E,\mathrm{eV}) = f(E) - f(E+\mathrm{eV}), \qquad (11)$$

with the Fermi function $f(E) = \left(e^{\beta E}+1\right)-1$ and $\beta = \left(k_B T\right)^{-1}$. The Fermi function is the difference between charge distributions before and after transport [18,19]. The driving force here is the electric potential bias. Figure 4 shows the I-V characteristics of the metal/C_{60}/metal system for temperatures T=3K (dashed curve) and T=300K (solid curve), respectively. The dashed curve shows clearly a nonlinear dependence. Our results indicate a good qualitative agreement with the corresponding differential conductance illustrated in Figure 5. In other words, the low-voltage part of the dashed I-V curve arises from the semiconducting behavior of C_{60} molecule. On the other side, the increase of temperature crucially modifies this behavior (solid curve) and the I-V characteristic of the system shows a linear and ohmic-like behavior.

4. Summary and conclusion

Within a simple model, the effects of the electron-phonon coupling strength and the increase of the temperature on the electronic conduction and current-voltage (I-V) characteristics of C_{60} molecule in metal/C_{60}/metal system are numerically investigated. Our results indicate the conductance of the system decrease with the increasing of the electron-phonon coupling strength. In addition, the I-V characteristics of C_{60} molecule suggest that as the temperature increases the steps in the lower temperature curve of the I-V characteristic will be smoothed and the room temperature I-V characteristic of the system moves toward having an ohmic-like behavior while it exhibits a very considerable value of the differential conductance at room temperature.

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