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Room Temperature Conductance of Graphene Sheet as a Function of Some Variables Using LAD/SZ Method

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Abstract
Current study deals with the room temperature conductance of Graphene Sheets as a function of their binding energy and lengths. The structural properties of each sheet were calculated after the relax of the structures by performing the SIESTA-trunk-462 program. The results showed that the electric conductivity is inversely proportional to the theoretical separation of the gold electrode. The increase of the angle C-C-Au effects on the electric properties of the Graphene Sheet, the Sheet is became much conductive and effectient electrically at large angles. This may refers to that the electron transmission coefficient of the Graphene Sheet depends on the type of the contact of the top gold atoms of the pyramids with the anchor atoms in the Sheet.

Introduction

Graphene is a two-dimensional one-atom thick carbon sheets with a similar benzene-ring structure, has attracted tremendous interest among researchers from different fields, due to its outstanding physiochemical properties, such as a large specific surface area (2630 $m^2 g^{-1}$) [1], high-speed electron mobility (20000 cm^2 Vs) [2], excellent thermal conductivities (5000 W m^{-1} K^{-1}) [3], and well electro catalytic activity [4]. Graphene is an excellent conductor, it is not a metal but rather a zero-gap semiconductor. While the valence and conduction bands do not overlap in graphene, they touch at the Fermi level [5-7]. Graphene is an atomic monolayer of graphite [8] is a gapless semiconductor with linear electron spectrum [9]. In recent years, graphene and its derivatives were used to assemble into kinds of carbon-based materials, for instance, one-dimensional tube-in-tube nanostructures[10], two-dimensional layer stacked films[11-13] and three-dimensional graphene hydrogels [14-17] and aerogels [18-22].

Theoretical Methods and Computational Details

The electrical conductance of the studied Graphene Sheets was calculated using Density functional theory at local density approximation/single zeta LDA/SZ basis sets method. The LDA/SZ has shown to be highly successful for calculation the electronic properties such as ionization potentials, electron affinity, fermi energy, electrochemical hardness, electronic softness, electronegativity and energy gaps [23-27]. The DFT partitions the electronic energy are the electronic kinetic energy, the electron nuclear attraction and the electron-electron repulsion terms, respectively. The relax of the structures is done using the SIESTA – trunk - 462 program [28] and the calculations were carried out using the GOLLUM program " version 1.0 " [29].
The room temperature electrical conductance G was computed from the formula[30-32]:
Where is the Fermi function, $\beta=1/k_BT$, E_F is the Fermi energy and
is the quantum of conductance[32].
Since the quantity is a probability distribution peaked at $E=E_F$, with a width of order kBT, the above expression shows that G/G0 is obtained by averaging T(E) over an energy range of order k_BT in the vicinity of $E=E_F$.

Results and Discussion

Figure(1) shows the structures of the Graphene Sheets GR-1, GR-2 and GR-3 relaxed at the minimum energy. The optimized parameters of all studied structures included the bonds between two atoms in A^0 and angles in degree showed that the values of the bonds C-C, C=C and C-H are (1.451, 1.445 and 1.181) A^0, respectively, and C-C=C is 1.221^0, the optimized parameters are remain independent of the length of Graphene Sheet and agree with those for carbon rings structures[33,34]. This an indication to good relax done by employing LDA/SZ method. The calculations of bonds and angles of pure Graphene Sheets referred to that these papers keep their symmetrical configurations through the plane of two-dimensions.

Figure 2 shows the relaxed junctions of the studied Graphene Sheets. The structural features of the relaxed junctions are illustrated in Table 1. d is the distance between C-C centers atoms. L is the molecular length, which is the center to center distance of the apex atoms of the two opposing gold pyramids in the relaxed structure. X is the bond length between the top gold atoms of the pyramids and the anchor atoms. Z is the theoretical electrode separation, which defined as $Z=d_{Au-Au}-0.25nm$, where d_{Au-Au} is the center to center distance of the apex atoms of the two opposing gold pyramids in the relaxed structure, and 0.25nm is the value of d_{Au-Au} when the conductance through the two contacting pyramids (in the absence of a molecule) is G_0. Θ° is the angle between C-C-Au terminal.

Table 2 shows the calculations of the room temperature conductance G/G0, the binding energy B.E and the total energy E_{Total} in eV as functions of the theoretical gold electrode separation Z in nm and the angle Θ◦. The calculations are done at $E_F - E_F^{DFT} = 0.5$ eV.

The conductance of the pure Graphene Sheet was increase with decreasing the binding energy of the structure, as seen in Figure 4. GR-3 of the lowest binding energy has the largest value of electric conductivity, this result is a reflection of the calculated values of total energy E_{Total} of the Graphene Sheets under study, in which the total energy is of order of GR-3< GR-2< GR-1, as in Figure 5. Figure 6 showed that the electric conductivity is inversely proportional to the theoretical separation of the gold electrode, increase this separation leads to decrease the electric conductivity of the Graphene Sheet. The reason of this result is that the larger the spacer of contact junction will become a resistance factor of quantum transport of electrons through the gold pyramid. The influence of the angle C-C-Au in the terminal ends on the electric conductivity calculations of the studied Graphene Sheets is shown in Figure 7. The increase of the angle C-C-Au effects on the electrical properties of the Graphene Sheet, the Sheet is became much conductive and effectient electrically at large angles. This may refers to that the electron transmission coefficient of the Graphene Sheet depends on the type of contact of the top gold atoms of the pyramids with the anchor atoms.

Conclusions

From the results, one can conclude that the calculations of the geometrical parameters of the studied pure Graphene Sheets referred to that these Sheets keep their symmetrical configurations through the plane of the two-dimensions. The electric conductivity is inversely proportional to the theoretical separation of the gold electrode, increase the theoretical separation leads to decrease the electric conductivity of the Graphene Sheet. In addition, the increase of the angle C-C-Au effects on the electrical properties of the Graphene Sheet, the Sheet is became much conductive and effectient electrically at large angles. So, the electron transmission coefficient of the Graphene Sheet depends on the type of contact of the top gold atoms of the pyramids with the anchor atoms in the Sheet.

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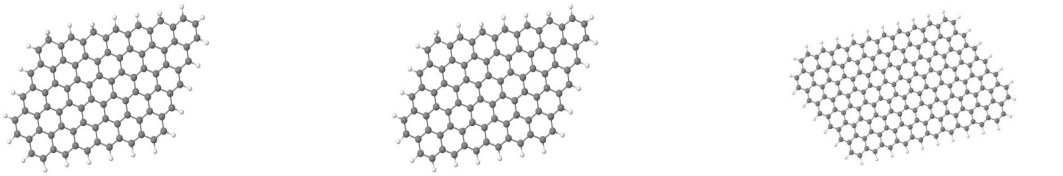
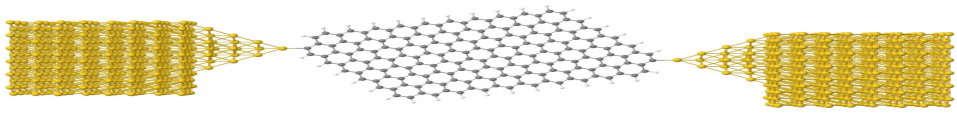
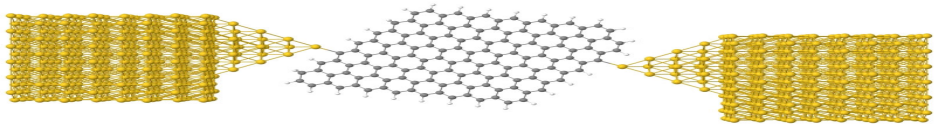


GR-1 **GR-2** **GR-3**

Figure 1. The relaxed molecules.



GR-1



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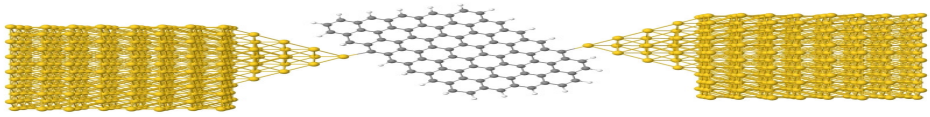

GR-3

Figure 2. The relaxed junctions

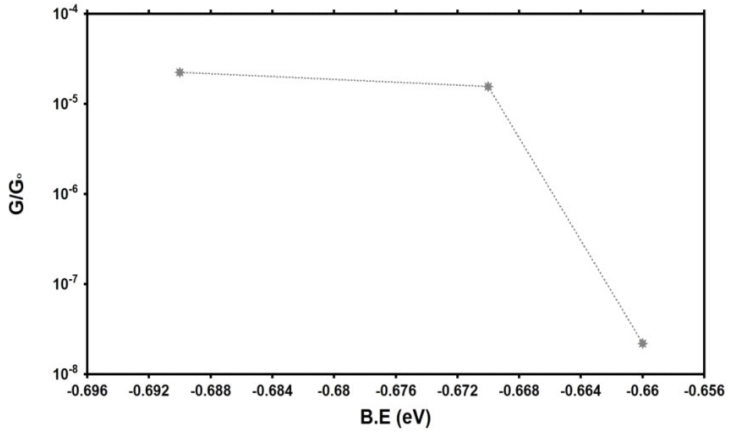

Figure 3. The room temperature conductance as a function of the binding energy for the Graphene Sheets at E_F-E_F^{DFT} = 0.5 eV.

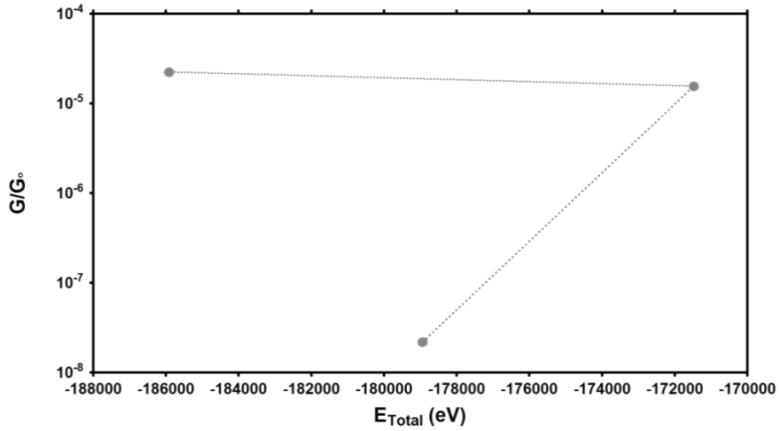

Figure 4 The room temperature conductance as a function of the total energy for the Graphene Sheets at E_F-E_F^{DFT} = 0.5 eV.

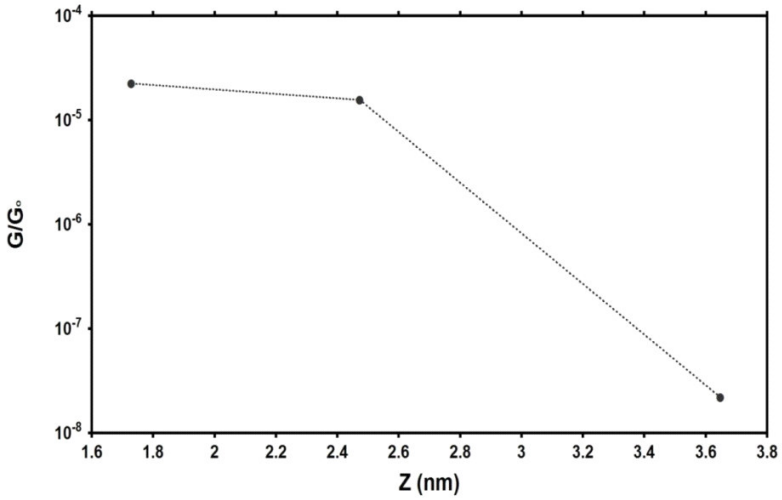

Figure 5 The room temperature conductance as a function of the theoretical electrode separation for the Graphene Sheets at E_F-E_F^{DFT} = 0.5eV.

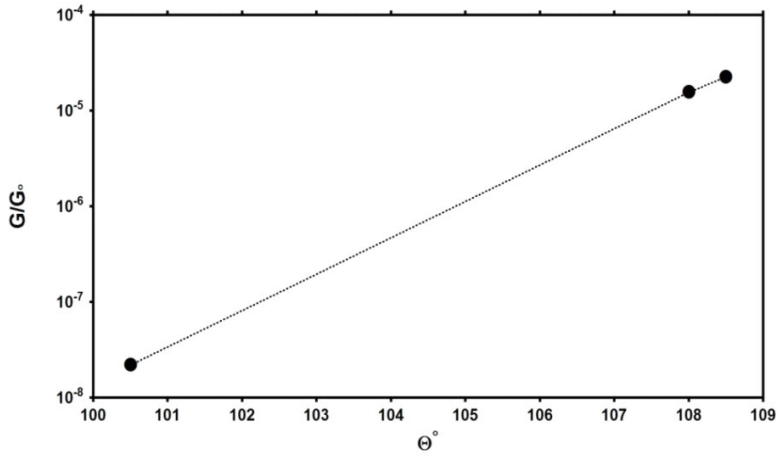

Figure 6. The room temperature conductance as a function of the junction configuration (C-C-Au terminal) for the Graphene Sheets at E_F-E_F^{DFT} = 0.5 eV.

Table 1. The structural features of the relaxed junctions.

Molecule	d nm	L nm	X nm	Z nm	Θ°
GR-1	3.410	3.898	0.245	3.648	100.5
GR-2	2.274	2.723	0.245	2.473	108.0
GR-3	1.531	1.979	0.245	1.729	108.5

Table 2. The room temperature conductance ($G/G_\circ$), the binding energy (B.E), the total energy of the system (E_{Total}), the angle between C-C-Au terminal (Θ°) for the studied Graphene Sheets

Molecule	E_{Total} (eV)	B.E (eV)	$G/G_\circ$	Z nm	Θ°
GR-1	-178942.217484	-0.66	2.02×10^{-8}	3.648	100.5
GR-2	-171476.397430	-0.67	1.56×10^{-5}	2.473	108.0
GR-3	-185914.164041	-0.69	2.24×10^{-5}	1.729	108.5