Quantum Transport Calculations For A Graphene Nanostructure Using Gold Electrodes

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Abstract. Ab intio quantum transport calculations based on the method of numeric localized atomic orbitals, pseudopotentials and Density Functional Theory have been performed, using SIESTA & TranSIESTA codes, for a graphene nanostructure using gold electrodes. Non equilibrium Green's Functions method have been used in conjuction with Density Functional Theory, as implemented in TranSIESTA, for calculations of transmission function, density of states and voltage-current characteristic. Transmission function and density of states show a discrete band structure which varies with applied voltage. In the voltage-current characteristic current shows non-linear fluctuating pattern with increase in voltage and lies in the pico-ampere range.

Keywords: Graphene, Transport properties, Density functional theory, SIESTA, TranSIESTA, Transmission Function.
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INTRODUCTION

Carbon based materials such as graphene (a single hexagonal structure of carbon atoms) have generated a lot of interest due to their exotic electronic properties [1-3]. Novel condensed matter effects arising from its unique two dimensional (2D) energy dispersion along with superior properties make it a promising material for next generation of faster & smaller electronic devices.

Study of transport properties of nano structures is current research interest [4-7]. In this paper we have performed first principle quantum transport calculations for graphene nano structure attached to gold electrodes using TranSIESTA [7, 8] which calculates transport properties using nonequilibrium Green's function approach. Transmission functions, electron density of states, projected density of states and current-voltage characteristic have been calculated (see Figure 1).

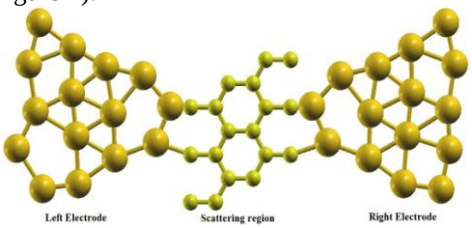


FIGURE 1. Schematic view of graphene nano structure along with gold electrodes. Central part is the scattering region, left and right parts are gold electrodes.

SIMULATION DETAILS

We have performed ab initio calculations within the framework of DFT as implemented in SIESTA code [8]. Troullier Martin, norm conserving, relativistic pseudopotentials have been used for both carbon and gold. The exchange and correlation energies are treated within the generalized gradient approximation (GGA) according to the Perdew, Burke and Ernzerhof (PBE) parameterization. Throughout the geometry optimization, numerical atomic orbitals with single zeta polarization (SZP) basis set with confinement energy of 0.01 Ry were used. The Brillouin zone was sampled using Monkhorst-Pack scheme with a 1×11×40 mesh for the calculations and 250 Ry mesh cutoff energy was used. An interaction between adjacent graphene layers is hindered by a spacing of 20 Å. The scattering region consists of a graphene nano structure containing 18C atoms in the form of 3x3x1 super cell. The electronic transport properties are studied by the nonequilibrium Green's function techniques, within the Keldysh formalism [9], based on density functional theory as implemented in the TranSIESTA module within the SIESTA. The current through the contact region has been calculated using Landauer-Buttiker formula [10]

$$I(V_b) = G_0 \int_{\mu_R}^{\mu_L} T(E, V_b) dE$$

Where $G_0 = 2(e^2/h)$ is the unit of quantum conductance and $T(E, V_b)$ is the transmission probability of electrons incident at an energy E through the device under the potential bias V_b. The electrochemical potential difference between the left and right electrodes is $eV_b = \mu_L - \mu_R$.

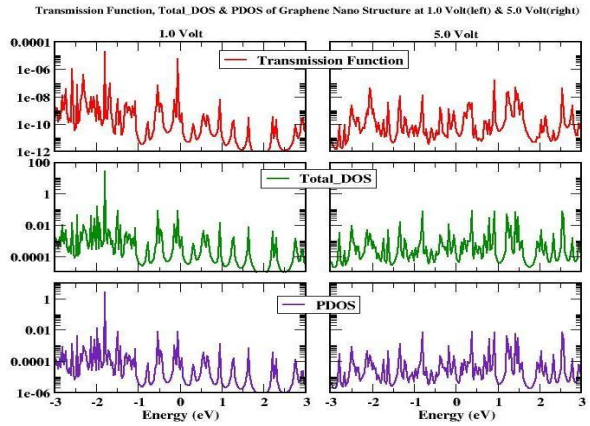
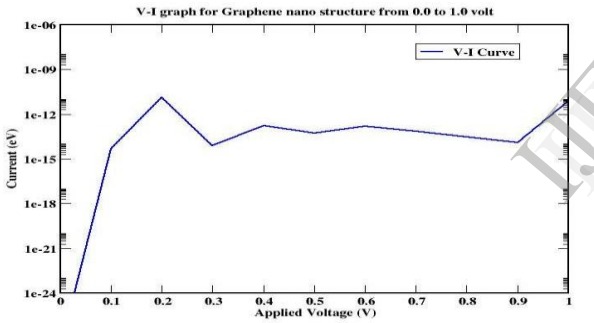
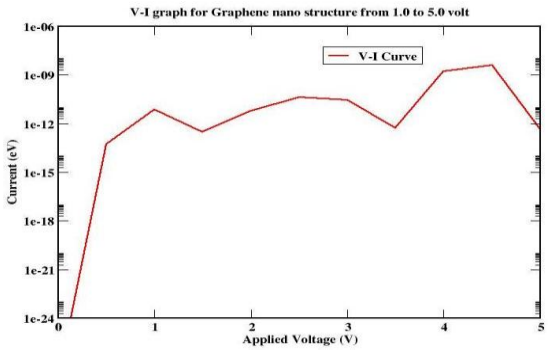


FIGURE 2. Transmission function, total density of states (DOS) and projected density of states (PDOS) of Graphene Nano Structure at 1.0 V and 5.0 V.



(a)



(b)

FIGURE 3. Voltage-Current (V-I) characteristics for graphene nano structure (a) for applied voltage 0.0 V to 1.0 V at 0.05V steps (b) for applied voltage 0.0 V to 5.0 V at 0.25 V steps.

RESULTS AND DISCUSSION

Figure 2 shows the transmission function, total density of states (DOS) and projected density of states (PDOS) of Graphene Nano Structure at 1.0 V & 5.0 V.

It is clear that the transmission function, projected density of states and total density of states show a discrete band structure which varies with applied voltage

Figure 3 (a & b) shows the Voltage-Current (V-I) characteristics for graphene nano structure. It is observed that in the V-I characteristic current shows non-linear behavior fluctuating with the change in voltage.

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