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**Short Communication**

**Theoretical computation of the quantum transport of zigzag mono-layer Graphenes with various z-direction widths**

**ABSTRACT**

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The quantum transport computations have been carried on four different width of zigzag graphene using a nonequilibrium Green's function method combined with density functional theory. The computed properties are included transmittance spectrum, electrical current and quantum conductance at the 0.3V as bias voltage. The considered systems were composed from one-layer graphene sheets differing with each other in y-direction width. The number of unit cells for considered graphenes are one, three, five and seven in z-direction, while the scattering region and first super cells of semi-infinite right and left electrodes were formed from three unit cell in z-direction. At the first the considered structures have been optimized and next the NEGF calculations were carried out on the optimized structures. All of the computations have been done using OPENMX3.6 atomic scale simulation code. The results were presented and interpreted for the considered systems in terms of the z-direction width of studied graphenes.

**Keywords:** *NEGF; Graphene; Quantum Transport; DFT; Conductance.*

**INTRODUCTION**

Development in experimental fabrication of a single layer of graphite (graphene) has led to drastic discovery of electronic properties and new quantum transport phenomena in this material, recently [1–7]. The graphene is attracting much interest for its novel physical properties [2, 3] and its possible applications as a candidate to future electronic devices [4, 5]. Its particular geometry (one-dimensional) caused to the graphene nanoribbons (GNR) used for practical applications in electronic devices. The electronic structures, electronic transport behaviors and optical properties for GNRs studied by doping, introducing defects, or chemical modification techniques [6–14]. Furthermore, several prototype electronic devices based on graphene nanoribbons have been manufactured in experiments [12, 13].

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Doping the GNR is a popular method to orient the physical properties of graphene [6, 14]. For example, doped graphene with boron and nitrogen can be used as a promising electrode for high-power and high-energy lithium ion batteries with high-rate charge and discharge moods [15]. Also, the doped graphene in some field effect transistor (FET) devices can display p-type and n-type characteristics<sup>16</sup> and it can display the FET feature when the edge carbons substituted by B or N atoms.<sup>14</sup> However, recently much attention is focused on disordered, random doping and both of them. It will be useful for the modified manufacturing and using pristine GNRs and novel transport characteristic [16,17].

The nonequilibrium Green function (NEGF) method [18,19] potentially has several advantages to investigate electronic transport properties of nanoscale materials such as single molecules, atomic wires, carbon-based materials, and thin layers [20-24].

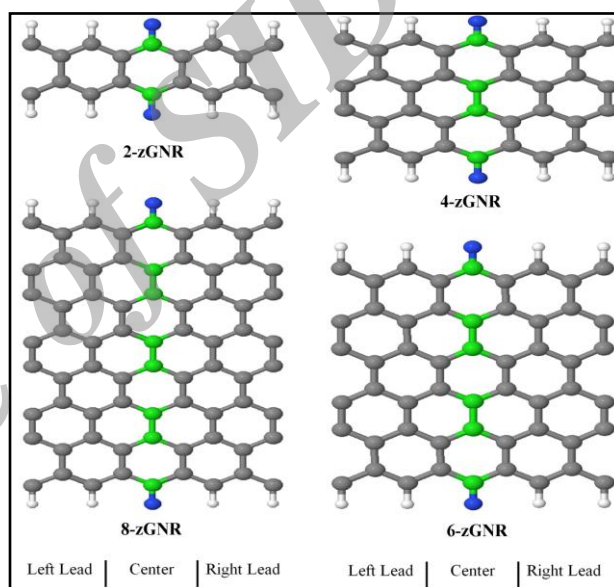
In this paper, we present a study of the electronic and transport properties of difference width of graphene nanoribbons consisting of two semi-infinite zigzag graphene nanoribbons by means of the non-equilibrium Green's function (NEGF) method combined with density functional theory. The transport properties of such junctions are investigated and are calculated at 0.3V as bias voltage.

## EXPERIMENTAL

### Computational Methods

The quantum transport calculation has been done for four different width of zigzag graphene nanoribbon (2-zGNR, 4-zGNR, 6-zGNR and 8-zGNR) that are shown in Figure 1. These open systems are constituted by three parts: the left lead (L) and right lead (R) semi-infinite graphene leads, and a center region (C) between them (green for carbons atoms and blue for hydrogen atoms in center region). For these systems unit vectors and unit cells are modified. The numbers of unit cells are one, three, five and seven in z-direction for 2-zGNR, 4-zGNR, 6-zGNR and 8-zGNR, respectively. While the scattering region and first super cells of semi-infinite right and left electrodes were formed from three unit cell in y-direction for

all studied structures. The electronic structure calculations are carried out using the first-principles self-consistent method implemented in the OPENMX3.6 package [25]. The exchange–correlation energy and electron–ion interactions are described by the Perdew–Burke–Ernzerhof (PBE) [26] generalized gradient approximation (GGA) and norm-conserving pseudopotentials [27] in the fully nonlocal form, respectively. A double-z polarized basis set of numerical atomic orbitals is used and the energy cutoff for real-space mesh is set to 150 Ry [25]. The electronic transport is studied with the Tran Main code, which combines the NEGF technique with density functional theory.



**Fig. 1.** Configure of the left and right leads and center region for 2-zGNR, 4-zGNR, 6-zGNR and 8-zGNR.

## RESULTS AND DISCUSSION

We first optimized the 2-zGNR, 4-zGNR, 6-zGNR and 8-zGNR structures using openmx3.6 package and double-z polarized basis set of numerical atomic orbitals. Then the density of states (DOS) and HOMO-LUMO energy states were calculated for any studied structures. The aim of these calculations was to achieve the conductivity from the differences of the HOMO-LUMO energy states gap. Furthermore, the transmittance, conductance and current were calculated for any studied structure at 0.3V as bias voltage. The current and conductance vs. four

studied structures curves are shown in Figure 2. The conductance curve is showed 2-zGNR has highest and 6-zGNR has lowest conductivity and are  $3.817084$ ,  $0.03027805G_0$ , respectively. The order of increasing of conductivity for these structures is

$$2\text{-zGNR} \gg 4\text{-zGNR} > 8\text{-zGNR} > 6\text{-zGNR}$$

So, it can be a special characteristic for 2-zGNR which has highest conductivity and this difference is observable. Also, as can be seen from current curve the order of increasing for currents at  $0.3$  V as bias voltage is almost the same as the order of conductivity increasing order and 2-zGNR has highest and 6-zGNR has lowest current at  $0.3$  V as bias voltage and are  $30.69844$ ,  $3.750576$  micro ampere, respectively. The order of increasing for current is

$$2\text{-zGNR} \gg 8\text{-zGNR} > 4\text{-zGNR} > 6\text{-zGNR}$$

The Transmission spectrum at  $0.3$  V as bias voltages for 2-zGNR, 4-zGNR, 6-zGNR and 8-zGNR were shown in Figure 3. As can be seen, by increasing the widths of graphene nanoribbons intense of the spectrums have been increased. It can be reasonable because when the widths of graphene nanoribbons increase the channels or states for transition electrons are increase, so probability for transition of electrons with certain energy witch equal the transmission spectrums intense are increase.

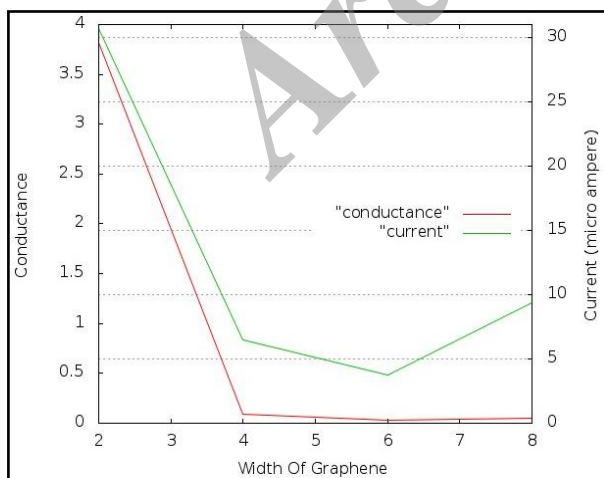


Fig. 2. The conductance and current curve for 2-zGNR, 4-zGNR, 6-zGNR and 8-zGNR at  $0.3$  V as bias voltage.

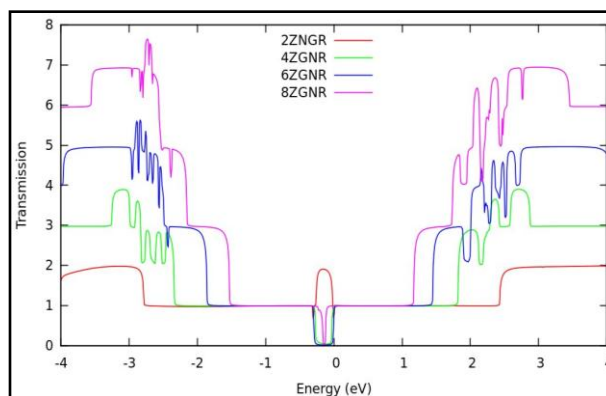


Fig. 3. The transmittance spectrum for 2-zGNR, 4-zGNR, 6-zGNR and 8-zGNR at  $0.3$  V as bias voltage

## CONCLUSIONS

We have investigated the electronic structures and transport properties of four difference width of zGNR. The width of GNR can obviously tune the transmittance of the graphene nanoribbons. The energy dispersions, band gaps, DOS and probability transmission depend sensitively on the geometry and the width of the graphene nanoribbon. The numbers, heights, and energies of the DOS peaks are dependent on the width of zGNR. The reason for all observations can be that the increasing the width of zGNR causes the electron transfers between different sub lattices (between leads and center region) and among different atoms within the same sub lattice (through lead or center region) be ease, and increase the probability transmission noticeably.

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