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Research Article

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Electron Transport in N-doped Graphene Nanoribbone

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Abstract The metal-to-semiconductor progress has been seen in graphene nanoribbons (GNRs) with a different novel electronic and auxiliary attributes. The planned and extent of GNRs for a variety of suggestions could be spread altogether by this change. In light of powerful utilitarian hypothesis (DFT) computations, it considered the transport properties of armchair GNRs doped with nitrogen (N) alongside various edge morphology. Armchair nanoribbons are known to display metallic conduct without utilizing turn. The auxiliary properties, in particular, edge state, doping and lace width, can be considered to influence the electronic properties of GNR structures. In this examination, the adjustments in the electronic properties by doping a N particle with different nuclear rates (16.6%, 33.3% and 55%) were researched. Estimations were finished by utilizing the neighborhood thickness guess self-consistent-charge tight-binding (SCC-DFTB). Within the sight of exceptional edge expresses, the edge-adjusted frameworks show a perceptible change with unmistakable and better N versatility. Thus, it has been seen that subbing two N particles at the carbon edges is increasingly overwhelming contrasted with other doping designs. We expect that our impossible to miss results will have potential applications in vitality change, sun oriented cells and thermoelectric gadgets.

Keywords Graphene nanoribbons, electronic structures, transport properties, N-doping

Introduction

The high electron portability and long lucidness length make graphene a subject of incredible enthusiasm for nanoscale hardware applications [1]. Be that as it may, the principle issue in the advancement of graphene based field impact transistors is the failure to electro-statically limit electrons in grapheme [2-4]. This is on the grounds that a solitary layer of graphite remains metallic even at the charge lack of bias point. Because of that issue, an approach to open a gap in electronic structure of graphene must be found [5]. The two-dimensional graphene has pulled in a lot enthusiasm because of its exceptional electronic just as transport properties portrayed by massless Dirac condition [6]. A decent number of writing is accessible in both exploratory also, hypothetical investigations comprehend the electronic, transport, and optical properties of graphene. Slender graphene strips (GNR) are created and anticipated to majorly affect their electronic vehicle properties. The electronic properties of GNRs are basically subject to the width and nuclear geometry of their edge by opening a band gap, to be specific, zigzag or armchair. Perspective on the enthusiasm for the examination of edge states of the electronic structure of zigzag graphene nanoribbons (ZGNRs), they display promising potential applications in spintronics [7-11]. Energy gap can be tuned from multiple points of view. To open the energy gap of graphene, a few techniques, for example, heteroatom doping, functionalisation, application of electric field and keeping graphene on substrates like SiO_2 and SiC have been proposed [12,13]. Later improvements on graphene have focussed on fitting its properties by subbing heteroatoms or making opportunities in the cross section of graphene. Electron and opening co-doping is a conspicuous technique to open the energy gap around the Fermi level in graphene while B and N co-doping are the well-known decisions in graphene N-doped graphene has a metallic nature, thus it shows an expanded reactivity toward free radicals as watched for metallic nanotubes too

[14-16]. In this paper, it has planned a structure to balance the electronic transport of graphene by utilizing extraordinary convergences of N with zigzag edges, having a strip width of NZ = 6, in light of the primary guideline computations in which N goes about as the electron dopant.

Computational Method

Computations of geometrical optimizations, electron transport are performed by using the DFTB module implemented in Materials Studio software suite 7.0 (Accelrys Inc.). Periodic boundary conditions are used and the inter-graphene distance was kept to a minimum of 50 Å to avoid lateral interactions. The zigzag edges are fully passivated with hydrogen atoms. Figure 1 shows the unit cell of ultrathin ZGNR that used in this work. The ZGNR indicates doping positions labelled as one N atom case (N1), two N atoms case (N1and N6) and three N atoms case (N1, N3 and N5) as shown in figure 2. The geometry optimization was performed by using self-consistent-charge tight-binding (SCC-DFTB). The Slater–Koster parameter file mio was employed in SCC-DFTB part of the calculations. The structures of the GNRs studied here are fully relaxed according to the forces and stress on the atoms using the conjugate gradient minimization until the maximum force tolerance being less than 0.02 eV/Å. Finite temperature Fermi smearing is used to control electron state population near to the Fermi level with temperature kT=0.001 Ha. The self-consistent calculations are performed with a charge mixing amplitude of 0.2, and the SCC tolerance is taken as 1×10^{-5}.

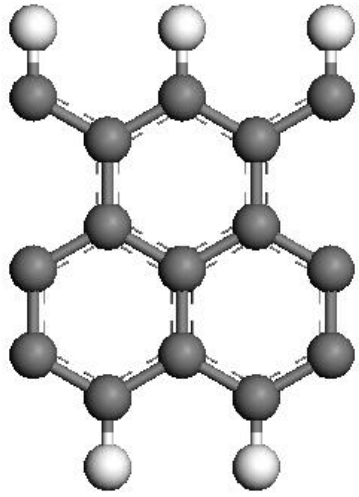

Figure 1: The unit cell of ultrathin ZGNR

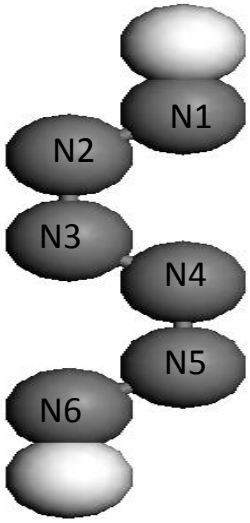

Figure 2: Atomic structure of the ZGNR

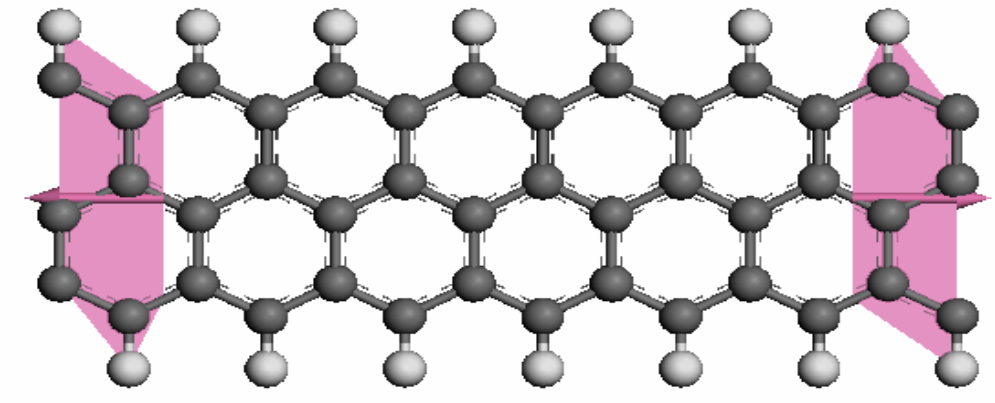

Figure 3: Atomistic scheme of the two-probe system of a ZGNR on the right and left edges of the scattering region

To perform reliable simulations, the transport calculations are carried out within the framework of density functional theory based SCC-DFTB combined with nonequilibrium Green's function (NEGF) method. The central channel region is sandwiched in between the left (source) and the right (drain) AGNR electrodes with the same width as the channel and the semi-infinite length. A two-probe system made of two principal layers, a schematic device is shown in Figure 3. The SCC-DFTB Hamiltonian is used to calculate the transmission coefficients T(E, V), and the current-voltage characteristics were calculated using the Landauer-Buttiker formalism. A k point separation of 0.02 yields a good balance between computational time and accuracy in the results.

Results & Discussion

The anticipated transmission is assessed so as to explore the electronic transport behavior in the N-doped ZGNRs. In figure 3, transmission coefficients as the function of energy with various edge morphology for undoped and N-doped graphene are appeared. For all cases, the transmission spectra are gotten from the energy extend from −4 eV to +4 eV. The determined zero bias transmission spectra for pristine ZGNR are outlined in figure 4. At balance, it very well may be seen from the transmission spectra for unblemished ZGNR that the transmission coefficient is a whole number and furthermore that there is a top of the very region of the Fermi level.

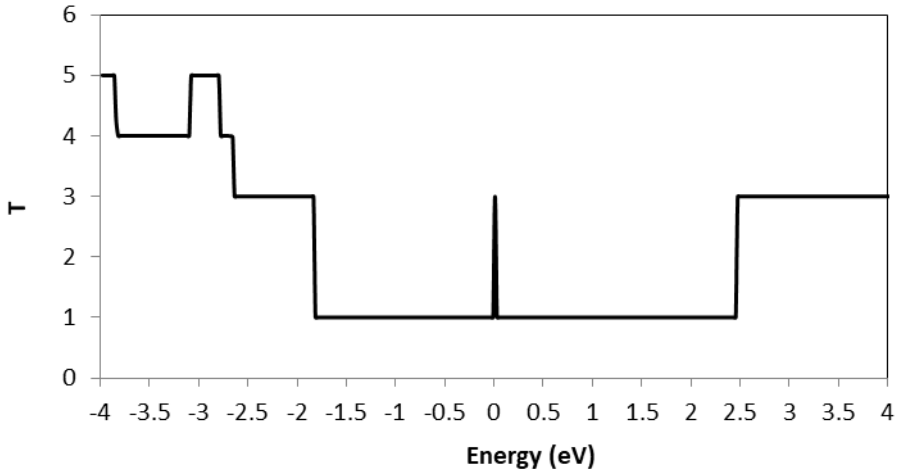

Figure 4: Transmission spectrum for the pristine ZGNR

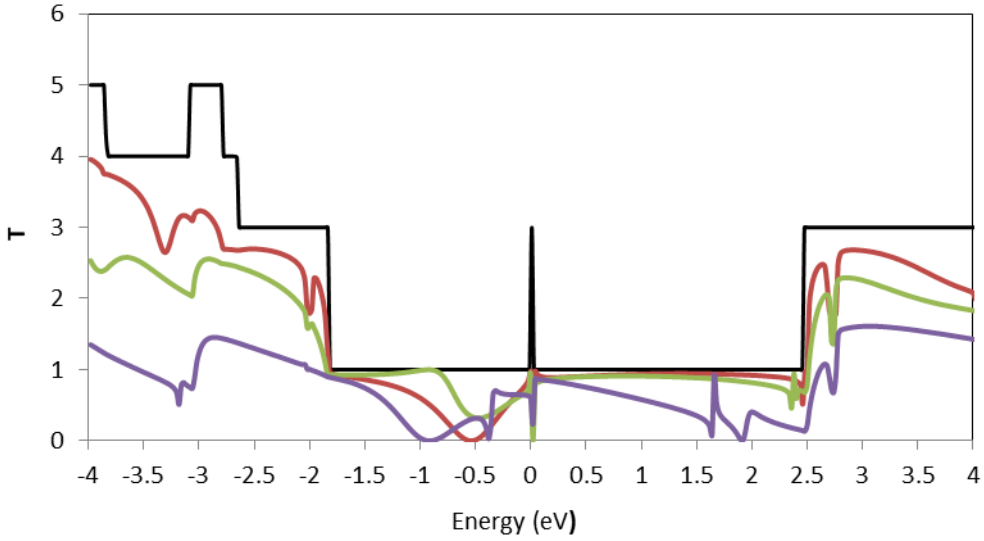

Figure 5: Transmission spectrum for the pristine ZGNR and ZGNR doped with N at different sites

Thinking about all doping designs as shown in figure 5, the transmission coefficient for all N-doped ZGNR is less contrasted with the immaculate ZGNR, which is brought about by the dissipating of the electrons by the doped N atoms. As the doping site changes, the transmission coefficient at a similar vitality displays a variety of all designs. It has watched some swaying conduct of T(*EF*) around *EF* = 0.3 eV, which can be ascribed to the band covering at these energies. Moreover, we can derive from figure 5 that the motions will in general be more stunning when doped with two N molecules at the upper and lower edges, which is affirmed by the band structures.

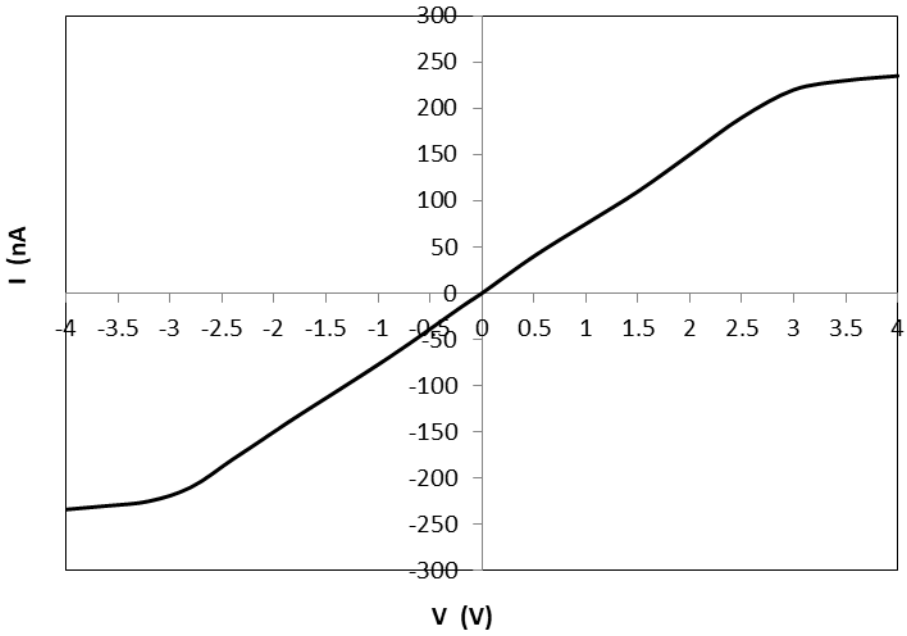

Figure 6: Current-voltage characteristic of pristine ZGNR

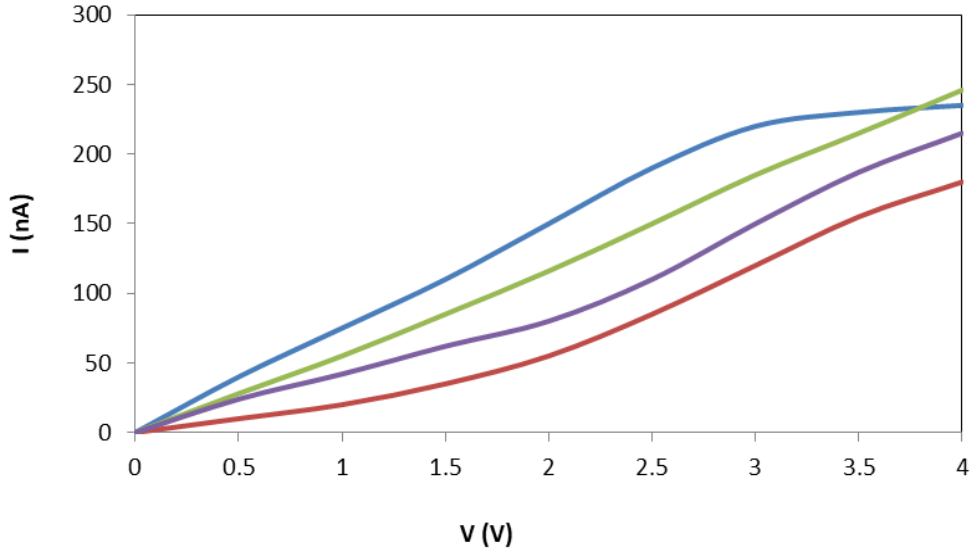

Figure 7: Current-voltage characteristic of N-doped ZGNR

Symmetric ZGNRs behave as conventional semiconductors in the presence of a conductance gap around the Fermi level, and exhibit unexpected threshold current-voltage dependence with very small currents. The Current-Voltage (I-V) characteristics of the structures, which is compared between each other, were studied by applying the voltage between 0.0V and 1.0V as shown in Figure 8. From the curves obtained it is observed that the graphene nanoribbons exhibit an interesting behavior. As shown clearly, the current in each device begins to flow at a different bias voltage, and the threshold of the junctions is sensitive to the length and charge state of

the embedded ZGNR. This changed threshold voltage implies that the existence of structural effects on the transport energy gap. Reflecting the distributions of the transmission functions, the electron transport property is semiconductor like conductivity. With the bias increasing, both of HOMO and LUMO extend gradually to the Fermi level and overlap at threshold bias voltage. Unambiguously, it is the overlap between HOMO and LUMO that forms the first transport channel in the perfect ZGNR. Thus, the current starts to flow at this point.
As a result, the current increases with the increase of the applied voltage as shown. With the increase of bias larger the threshold, the I-V curve presents a linear growth trend. The dependence of the Dirac electron tunneling current on the source voltage for different ZGNR lengths is depicted in Figure 9. As a result, the Dirac electron tunneling current decreases. In the case of nanoribbon N1, for low bias voltages, current flow is ohmic. As the voltage bias is increased >2.5 (V), at a particular voltage (cut-in voltage), conduction saturate and a linear curve is obtained there on.

Conclusion

The transport properties of short ultrathin N-doped ZGNRs with different concentration have been systematically investigated, using a nonequilibrium Green's function formalism in combination with density functional tight binding method. Without spin, pristine ZGNR terminated with H atom shows metallic behavior while the initial-scaled spin ZGNR is semiconducting, i.e. antiferromagnetic. It has observed that the position of dopant atoms plays a crucial role in engineering the transmission spectra and current-voltage characteristic. Depending on the N concentration, we observed the semiconducting behavior for the 2N case, whereas it exhibits metallic behavior with the other doping concentrations.

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