

Transport properties of asymmetric zigzag graphene nano-ribbon built by carbon vacancy in edge

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Abstract. Using nonequilibrium Green's functions in combination with density functional theory, we investigated the electronic transport behaviors of single layer zigzag graphene Nano-ribbon (ZGNR) with a Carbon vacancy in edge. The results show that electronic transport properties of the asymmetry ZGNR can be modulated by vacancy in edges, and prominent negative differential resistance (NDR) can be observed. These results may be useful for designing practical devices based on graphene Nano-ribbons.

1. Introduction

Since the experimental synthesis of stable single graphene layer at room temperature was achieved, graphene has been the subject of numerous experimental and theoretical investigations due to the high electron mobility and the potential for sizing the electronic devices to nanoscales [1]. In particular, much effort is focused on obtaining graphene nano-ribbon (GNR) with tailored properties that could be key elements in future electronic applications. Two basic nano-ribbons are mostly studied, which are the edge of GNR pointing along the C-C bond referred to as the armchair GNR, and the edge perpendicular to the C-C bond referred to as the zigzag GNR.

It is well known that the C atoms of GNR are sp^2 bonded. Hence an edge atom would have dangling bonds, which would be saturated by atoms or molecular species. Recently, much research have been done concerning the modification of edges because it can be used to control the electronic properties of GNRs for different purposes. The sp^3 bonded edge atoms with 2H atoms at the edge can be stabilized over 1H atom terminated edge at high temperatures and pressures.

In this paper, we present a theoretical description of transport properties of a 6-ZGNR, including vacancy in edge in order to show its impact on the whole structure's conductivity. The geometrical structures of two primitive (one Carbon and its adjacent hydrogen at edge picked up) and its relaxed and optimized models have been shown in figure 1. The electronic transport properties have been studied by the first-principles calculation, differences compared.

As shown in figure 1. (a)-(b), the model configuration, called 6-ZGNR in some previous references, are outstandingly differ from each other specifically in edges.



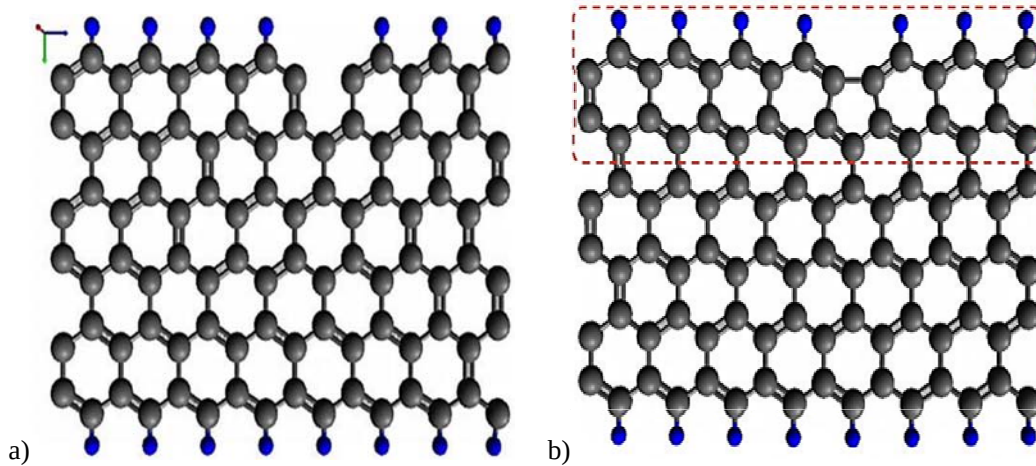


Figure 1. The geometry structure of a single layer zigzag graphene nano-ribbon passivated by Hydrogens when it (a) lacks of Carbon at edge (b) is relaxed and optimized.

2. Computational method and details

Transport calculations are based on density functional theory (DFT) combined with, nonequilibrium Green's function (NEGF) with SIESTA package. In our calculations, the vacuum layers between ZGNRs in neighboring along x and y directions (defined in figure 1) are 20 Å. The Perdew-Zunger exchange and correlation function within the generalized gradient approximation (GGA) is used. A cutoff energy of 350 Ry and a Monkhorst-Pack k -mesh of $1 \times 1 \times 12$ are chosen and double- ζ plus polarized basis set is adopted for electron wave function which has been proved to be capable of well describing the π -conjugated bond system and the transport calculation including transmission and current-voltage characteristics [2]. Geometry optimization is performed until the force is less than 0.001 eV/Å. The NEGF-DFT self-consistency is controlled by a numerical tolerance of 10^{-4} eV. The electron temperature is set to 300 K in the transport calculations.

3. Results and discussion

Calculating band structure, we find the small negative direct band gap, which refers to conductivity of the structure, as shown in figure 2. Hence, we focused on central atoms in scattering region as shown in figure 3. First and foremost, we analyzed the total density of states of scattering region which as shown in figure 4 indicates outstanding number of states to be occupied in some intervals of energy, compared to their neighbors.

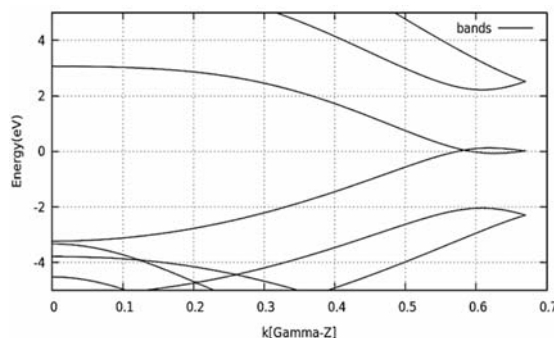


Figure 2. Band structure in $\Gamma - Z$ direction. 0.004Å transversal distance between conduction and valence bands indicates strong approximation of direct band gap, besides its -0.193 eV energy gap.

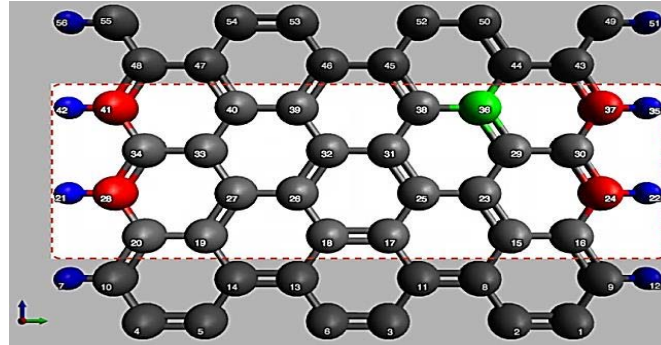


Figure 3. Scattering region focused on central atoms. PDOS of red (Carbons at edges) and green (Carbons in the middle) Carbon has been calculated.

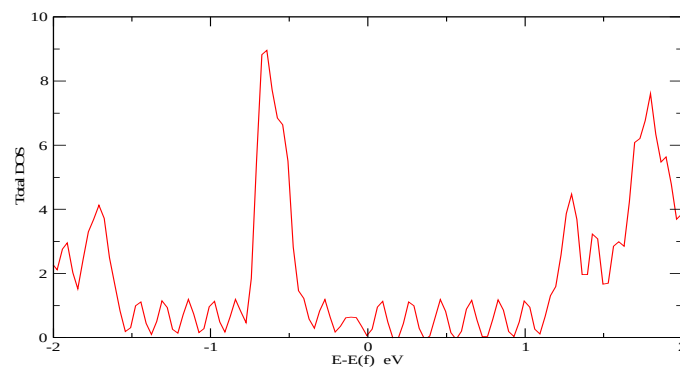


Figure 4. Total density of states (DOS) of the entire scattering region.

We studied the central atoms in more details, i.e. looking up the behavior of spin DOS for specific atoms depending on their positions. Except Carbons at edges, all the other Carbons in the middle of the scattering region have same treating in their spin DOS for different spatial directions and orbitals, as shown in figure 5. (Atom #36 in figure 3 is the green one which all the other middle Carbons have the same behavior).

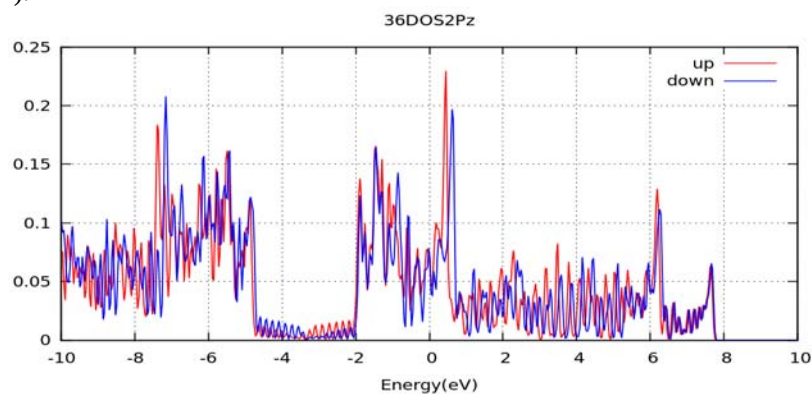


Figure 5. Partial spin DOS for different orbitals for central scattering Carbons.

When we calculated PDOS for edge Carbons, we figured out interesting spin separation in their DOS indicating which one does conducting more, shown in figure 6. Finally we computed the spin kind of I-

V characteristics for perfect and defect structure in figure 7, showing reduction in conduction in defect one and of course negative differential resistance (NDR), although totally the current is much low because of the structure's geometry [3].

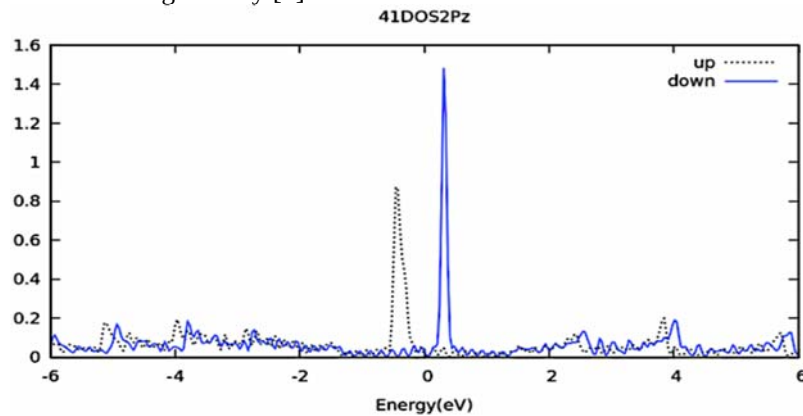


Figure 6. Atom #41 PDOS for orbital P in Z direction. All other edge Carbons (red ones) behave the same.

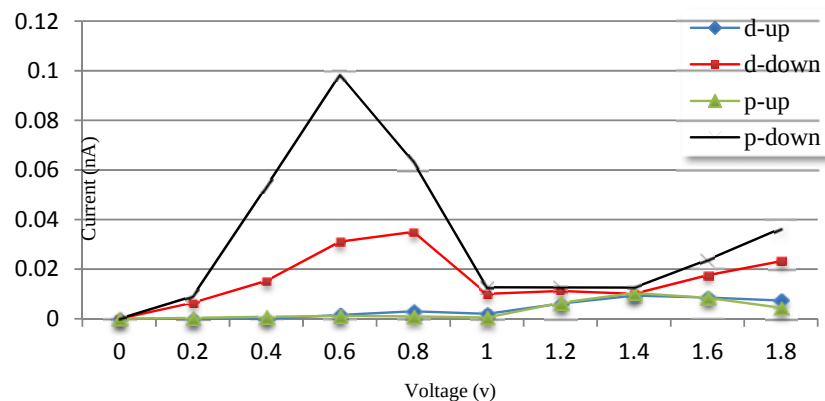


Figure 7. I-V spin graph of defect and perfect structures. Up spin current whether for defect one or perfect one has the same trending of current as voltage rising.

Since we observed spin filtering effect resulting from pdos polarization as shown in Figure 6, it leads us forward to using in spintronic devices. Besides, Negative Differential Resistance (NDR) which is showed in I-V curve is of great importance that occurred due to the electron tunneling into one of the neighboring islands (valleys) in conduction band i.e. into a system of states of reduced dimensionality. It means high energy electrons transmitting between two terminals don't have enough space (dimensional confinement) in collector (conduction band) so that they are tunneling to second barrier in collector and finally we observe decreasing current. Our results on transport properties of defected graphene and defect free graphene indicate a great potential in applications such as spin sensitive electronic devices.

References

- [1] Prins F *et al* 2011 *Nano Lett.* **11**(11) 4607-4611.
- [2] Kim W Y and K S Kim 2008 *Nat. Nanotechnol.* **3**(7) 408-412.
- [3] Li Z *et al* 2008 *Phys. Rev. Lett.* **100**(20) 206802.