Solid State Communications 227 (2016) 28–32

Contents lists available at ScienceDirect

Solid State Communications

journal homepage: www.elsevier.com/locate/ssc

The electron transport properties of zigzag graphene nanoribbons with upright standing linear carbon chains

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ARTICLE INFO

Article history:
Received 8 July 2015
Received in revised form
16 October 2015
Accepted 17 November 2015
by Y.E. Lozovik
Available online 22 November 2015

Keywords:
A. Graphene nanoribbon
D. Electronic properties
E. First-principles

ABSTRACT

The electron transport properties of zigzag graphene nanoribbons (ZGNRs) with upright standing carbon chains are investigated by using first-principles calculations. The calculated results show a significant odd-even dependence. The currents of even-numbered chain configurations are small because a suppression emerges around the Fermi energy in the transmission spectra under a finite bias. However the $I-V$ curves of odd-numbered chain structures display metallic properties with a big transmission peak in the transmission spectra, indicating the high conductance. These properties offer an interesting method by modifying the odd-even parity of the carbon chains to tune the electron transport properties of ZGNRS.

1. Introduction

Low-dimensional carbon-based nanostructures attract much attention owing to their great physical, electrical and chemical properties [1]. Graphene is a two-dimensional (2D) lattice of sp^2-hybridized carbon atoms. It is well known that graphene has high strength, extraordinary conductivity and excellent transmittance [2,3]. Graphene nanoribbon (GNR) is regarded as a quasi-one-dimensional (Q1D) structure, it can be cut from a graphene sheet [4–6]. Because of the reduced dimension of the ribbon, the edges of ZGNR are predicted to have a major impact on its electronic properties [7]. Kan et al. [8] have reported that the ZGNR shows half-metallic when it is edge-terminated by NO_2 groups at one edge and by CH_3 groups on the other side. As another kind of carbon structure, the linear monatomic carbon chain is considered as an ideal covalent one-dimensional (1D) system with *sp* hybridization. It is traditionally classified as cumulene (with double bonds, i.e, $=C=C=$) or polyyne (with alternating single and triple bonds, i.e., $-C\equiv C-$) [9]. Owing to its great potential applications in molecular devices, the 1D carbon chain is widely investigated by many researches. Recently, several groups have experimentally achieved the linear carbon chains through supersonic cluster beam deposition [10,11] and electronic irradiation [12,13]. For example, Jin et al. [14] have realized stable and rigid carbon atomic chains by removing carbon atoms row by row from graphene. In earlier researches, odd-even oscillatory conductance and rectifying behaviors were found in linear carbon chains. Qiu et al. [15] find that the current in odd-numbered chains is carried by resonances while that in even-numbered chains is mediated. Shen et al. [16] reported that linear ballistic transport is observed in odd-numbered chains but not in even-numbered chains. However in previous theoretical work, all the carbon atomic chains studied are in the direction of the electron transport, and the carbon chain itself is also the only way for the electron transmission. If the linear monatomic carbon chain is connected to the edge of ZGNR, being perpendicular to the direction of electronic transport, the chain will not be the main transport path. As the carbon chain is upright standing, it is interesting to investigate the influence of the chain on the transport of ZGNR. As far as we know, such a configuration has not been studied. Surprisingly, by performing the first-principles calculations we found the odd-even dependence of transport property still exist. The currents of even-numbered chain structures are small, a suppression emerges around the Fermi energy in the transmission spectra under a finite bias. While the $I-V$ curves of odd-numbered chain configurations show metallic behavior with high conductance, and a big transmission peak appears instead of a conductance gap. This phenomenon can be explained that odd-numbered upright standing carbon chains destroyed the symmetrical distribution of eigenstate in ZGNRs.

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http://dx.doi.org/10.1016/j.ssc.2015.11.013
0038-1098/

2. Computational method

We performed the first-principles calculations by the Atomistix Toolkit (ATK) package, which is based on the combination of density functional theory (DFT) and non-equilibrium Green's function technique [17]. The mesh cutoff energy is chosen as 150 Ry, and the *k*-point mesh is $1 \times 1 \times 100$ [18]. The Perdew-Burke-Eenzerhof formulation of the generalized gradient approximation (GGA) have been used as the exchange-correlation function, and the double-zeta polarized basis set is employed in the calculations. The size of the scattering region cell of bare ZGNR ($a \times b \times c$) is set to be $10.00 \times 20.00 \times 27.01$ Å^3, and the size of the electrode cell is $10.00 \times 20.00 \times 4.92$ Å^3. In our models, as the carbon chain length increases, the size of the *b*-axis direction of the central scattering area increases from 20.00 to 28.00 Å. In order to prevent the interaction with adjacent images, the vacuum spaces of supercell are set to be more than 10 Å. All the atomic positions of the structure have been optimized, until all residual forces on each atom are smaller than 0.02 eV/Å. The edges of ZGNRs are terminated with hydrogen (H) atoms to remove the dangling bonds. The two-probe device is divided into three parts: the left semi-infinite ZGNR electrode, the central scattering region and the right semi-finite ZGNR electrode (as shown in Fig. 1). The carbon chains are placed at the center of the scattering region edge, and contain N carbon atoms. In this study we choose N = 1 to 6 configurations to study, which are referred to C1–C6.

3. Results and discussions

In the C1–C6 models, the C1, C3 and C5 are odd-numbered chains configurations, and the C2, C4 and C6 belong to even-numbered chains structures. Through the structural optimization, we found that all the length of C-H bond remain to be 1.08 Å which are unchanged corresponding to that of bare ZGNR as shown in Fig. 2. The adjacent C-C bonds of even-numbered chains structures obviously differ in length, up to 0.19 Å, so their carbon chains' bonding pattern can be qualitatively assigned to alternating single and triple bonds showing obvious polyyne properties.

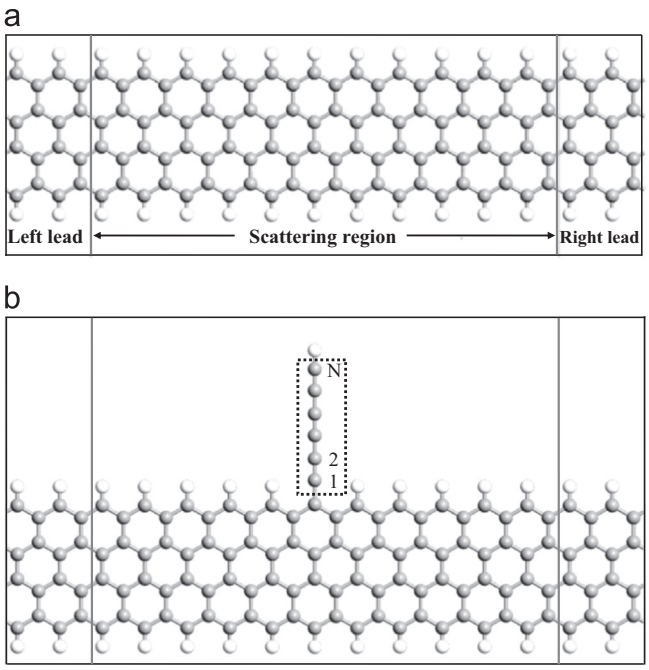

Fig. 1. Schematic illustration of (a) bare model; (b) CN model (N is the number of carbon atoms in the chain, from 1 to 6).

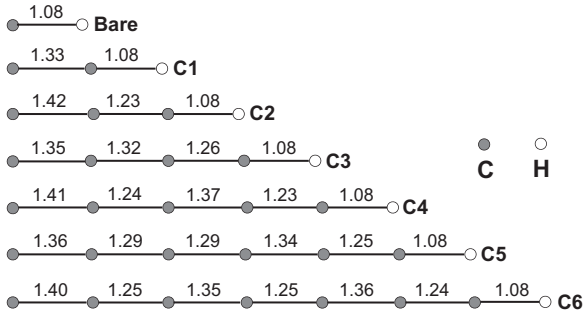

Fig. 2. Bond length of bare and C1–C6 configurations, in unit of Å. The left end of the carbon chain is connected to the ZGNR as shown in Fig. 1. For clarity, only the carbon chains are drawn, the ZGNRs are not shown here.

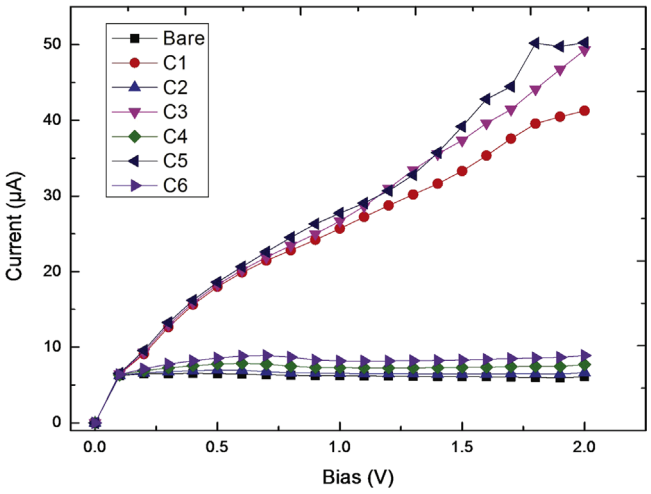

Fig. 3. (Color online) The current-voltage curves of bare and C1–C6 model in bias range from −2.0 to 2.0 V.

However, for odd-numbered chains, all the C-C bond lengths are similar, and these configurations are π-conjugated structures which present polyolefin properties [15,14].

The current-voltage (*I-V*) characteristics of all models are presented in Fig. 3. When the bias is below 0.1 V, all the curves are the same. However, as the bias increases, the shape of the *I-V* curves of even-numbered configurations are same as that of bare ZGNR. Only slight increase of the current with the increase of the chain length is observed. On the contrary, the currents of odd-numbered cases are larger than those of even models, and they increase when the bias increases, showing ohmic characteristics. So, we could conclude that the electron transport properties strongly depend on the chains's odd-even structure [19,20].

In order to investigate the physical origin of the odd-even characteristics in the *I-V* curves of these models, we first calculate their corresponding transmission spectra and the molecular projected self-consistent Hamiltonian (MPSH) under bias $V_b = 1.0$ V, as shown in Fig. 4. It can be found that, around the Fermi energy, odd-numbered configurations have three transmission peaks, however the even-numbered ones have an obvious suppression, which is similar to the bare ZGNR [Fig. 4(a) and (b)]. The transmittance spectra of the even-numbered models decrease distinctly in the range from −0.5 to 0.5 eV. To better compare their transmission spectra, we take C3 and C4 models as examples to study the electronic structure for odd- and even-numbered cases respectively. In Fig. 4(c), the highest occupied molecular orbital (HOMO), HOMO-1 and HOMO-2 locate below the Fermi level in the integral area, indicated by the shaded area. The lowest unoccupied molecular orbital (LUMO) lies on the right edge of the