Physics Letters A 380 (2016) 3198–3205

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Giant rectification in graphene nanoflake molecular devices with asymmetric graphene nanoribbon electrodes

Xiao-Li Ji, Zhen Xie, Xi Zuo, Guang-Ping Zhang *, Zong-Liang Li, Chuan-Kui Wang *

Shandong Province Key Laboratory of Medical Physics and Image Processing Technology, School of Physics and Electronics, Shandong Normal University, Jinan 250014, China

ARTICLE INFO

Article history:
Received 29 February 2016
Received in revised form 10 July 2016
Accepted 18 July 2016
Available online 22 July 2016
Communicated by R. Wu

Keywords:
Electronic transport property
Graphene nanoribbon electrodes
Carbon atomic chain
Graphene nanoflake
Nonequilibrium Green's function method

ABSTRACT

By applying density functional theory based nonequilibrium Green's function method, we theoretically investigate the electron transport properties of a zigzag-edged trigonal graphene nanoflake (ZTGNF) sandwiched between two asymmetric zigzag graphene nanoribbon (zGNR) and armchair graphene nanoribbon (aGNR) electrodes with carbon atomic chains (CACs) as the anchoring groups. Significant rectifying effects have been observed for these molecular devices in low bias voltage regions. Interestingly, the rectifying performance of molecular devices can be optimized by changing the width of the aGNR electrode and the number of anchoring CACs. Especially, the molecular device displays giant rectification ratios up to the order of 10^4 when two CACs are used as the anchoring group between the ZTGNF and the right aGNR electrode. Further analysis indicates that the asymmetric shift of the perturbed molecular energy levels and the spatial parity of the electron wavefunctions in the electrodes around the Fermi level play key roles in determining the rectification performance. And the spatial distributions of tunneling electron wavefunctions under negative bias voltages can be modified to be very localized by changing the number of anchoring CACs, which is found to be the origin of the giant rectification ratios.

1. Introduction

The motivation for miniaturization of electronic devices has driven an intensive research activity into nanoscaled and low-dimensional material systems. Graphene, a two-dimensional lattice of carbon atoms, has drawn widespread interest due to its unique electronic transport properties [1–4] and the potential technological applications since it was first synthesized successfully by Andre Geim and Konstantin Novoselov in 2004 [5]. The corresponding quasi-one-dimensional graphene nanoribbons (GNRs) can be obtained by conventional lithographic techniques in semiconductor industry. GNRs are recognized as the most novel and prospective materials in the carbon family for building new nanoscale electronic devices [6–9]. Many interesting physical properties based on GNRs, such as negative differential resistance (NDR) [10–14], rectification [15–17], spin filtering [14,16,18,19], field-effect characteristic [5,20], have been demonstrated. Two basic GNRs, armchair graphene nanoribbons (aGNRs) and zigzag graphene nanoribbons (zGNRs), are mostly studied. The properties of them are distinctly different. The aGNRs are semiconducting with the energy gap dominated by the width of the nanoribbon, whereas the zGNRs show metallic behaviors [1,9,21–23]. The graphene nanoflakes (GNFs), another important graphene derivatives produced by the geometric cutting of graphene along specific single crystallographic directions and functionalized with various edge modifications, have finite size with triangular, rectangular and hexagonal shapes. Among them, zigzag-edged trigonal graphene nanoflakes (ZTGNFs) are prominent in their electronic properties because of the existing of half-filled zero-energy states [24–26]. Additionally, linear carbon atomic chains (CACs) made of *sp*-hybridized carbon atoms, which also can be regarded as a family of graphene derivatives or extremely narrow GNRs, can be successfully carved out from graphene by using a high-energy electron beam [27–29]. For one carbon chain, two structures are traditionally available, polyyne (dimerized chains with alternating single and triple bonds, $\cdots$C–C≡C–C$\cdots$) and cumulene (monatomic chains with double bonds, $\cdots$C=C=C$\cdots$). For the chains with even carbon atoms, the polyyne is more favorable with lower energy, whereas for those with odd carbon atoms, the cumulene is more stable [30–33]. All carbon based materials, such as GNRs and GNFs, would have a strong coupling energy that favors electron transport. Thus, when molecular electronic nanodevices based on GNRs and GNFs are constructed, CACs are straightly adopted as their connections [12,19,34,35].

* Corresponding authors.
E-mail addresses: zhangguangping@sdnu.edu.cn (G.-P. Zhang), ckwang@sdnu.edu.cn (C.-K. Wang).

http://dx.doi.org/10.1016/j.physleta.2016.07.044
0375-9601/

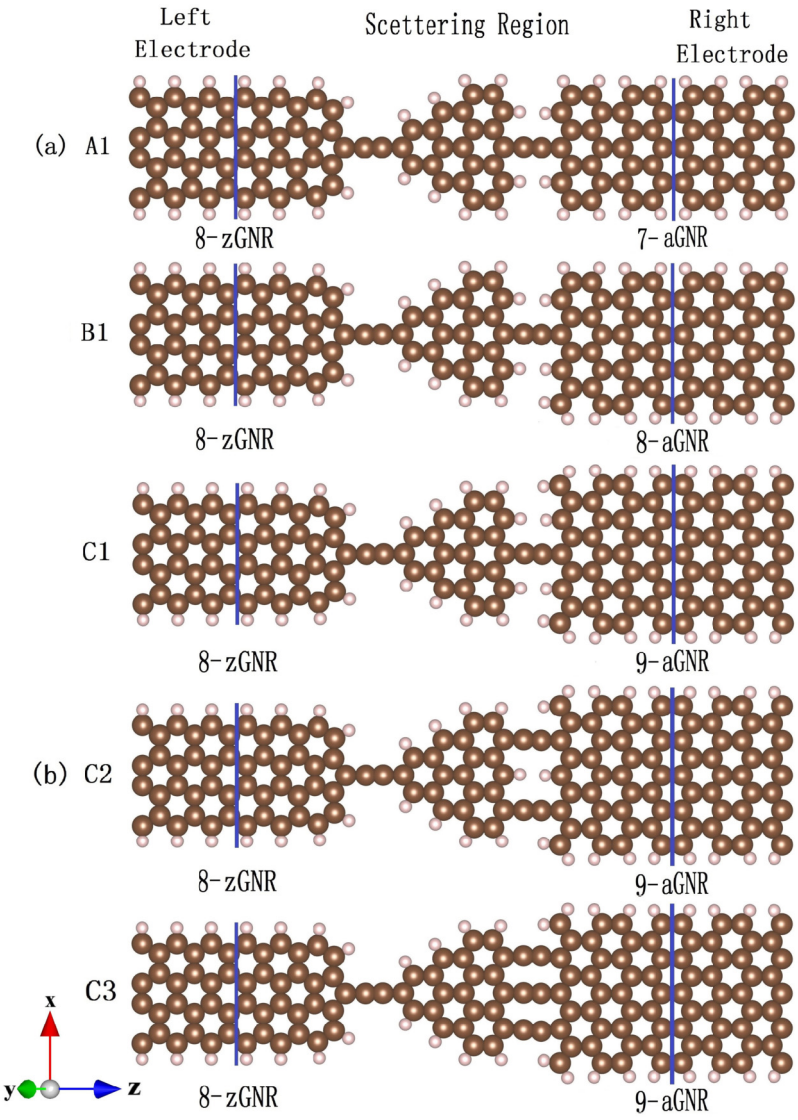

Fig. 1. Geometrical structures of the calculated molecular devices: (a) devices with the left 8-zGNR electrode and the right 7-, 8- and 9-aGNR electrodes are labeled as A1, B1 and C1, respectively; (b) the right connecting carbon atomic chain in device C1 is replaced by two, and three carbon atomic chains, and the corresponding devices are labeled as C2 and C3, respectively. The region between the two solid blue lines is the scattering region. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Our study showed that an asymmetric arrangement of aGNR and zGNR electrodes would lead to a marked rectification [34]. Zhang et al. have verified that ZTGNFs, when connected to gold electrodes by CACs, are very good candidates for designing rectifying devices [36]. More interestingly, the rectification direction can be modulated by varying the even-odd property of CACs. Up to now, gold electrodes are usually used in most studies of ZTGNF based electronic devices. However, complete carbon based devices, which are believed to be more promising in the subsequent integration, are still largely unexplored.

In this paper, we propose all-carbon based rectifying devices by connecting a ZTGNF to asymmetric zGNR and aGNR electrodes through CACs. Effects of the width of aGNR electrode and the number of connecting CACs are investigated to obtain large rectification ratio. Our calculations from the first-principles method show that the rectification performance of the devices is highly related to the width of the aGNR electrode and the number of connecting CACs.

2. Computational details

As shown in Fig. 1, the devices consist of three parts, one left 8-zGNR electrode, one right N-aGNR electrode and the scattering region. Here, 8 and N indicate the number of carbon atoms in the transverse x direction in the zGNR and aGNR, respectively. In the scattering region, a ZTGNF is connected to the left zGNR and right aGNR electrodes by carbon chains. Taking account of the influence of the carbon chain hybridization on the molecular device structure, we choose a three-atom carbon chain at the left side and a two-atom carbon chain at the right side as the connection carbon chains to keep the ZTGNF coplanar with the two GNR electrodes [34]. All the dangling bonds of edge carbon atoms are saturated by hydrogen atoms. The electron transport properties of molecular devices are highly related to the electronic states available around the Fermi level (E_F) and the anchoring groups bridging the central unit to the electrodes [37]. The aGNRs are semiconductors and the energy gap can be tuned by the width of the nanoribbon, therefore we investigate the effect of nanoribbon width on the electron transport and rectification properties of devices. Here, 7-aGNR, 8-aGNR, and 9-aGNR are used as the right electrodes and the corresponding devices are denoted as A1, B1, and C1 as shown in Fig. 1(a). Also, the number of CACs at the right side connecting the ZTGNF to the right 9-aGNR electrode is optimized to get large rectification ratios. And the rectification properties of devices