Physica E 95 (2018) 32–36

Contents lists available at ScienceDirect

Physica E

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

Effect of edge modification on the rectification in graphene ribbons device

Peipei Yuan[a], Xiaoxiao Han[a], Jingjuan Yang[a], Baoan Bian[a,*], Weibao Li[a], Yuming Wang[a], Xu Luo[a], Bin Liao[b]

[a] School of Science, Jiangnan University, Wuxi 214122, China
[b] College of Nuclear Science and Technology, Beijing Normal University, Beijing 100875, China

ARTICLE INFO

Keywords:
Molecular device
Electronic transport
Graphene rectifier

ABSTRACT

We perform first-principles calculations based on density functional theory and non-equilibrium Green's function to investigate the electronic transport properties of the 12-ZGNRs devices with edge modification of OH/NH_2, OH/NO_2 and OH/SO_2. The device with modified edge by OH/SO_2 shows the maximum (reverse) rectification ratio of 2076.33(1937.33). We discuss the effect of edge modification on rectifying phenomenon by calculating the transmission spectra and the energy band structures of the related electrodes as well as the PDOS at different bias. And the observed negative differential resistance effect is explained by the transmission spectra for device with modified edge by OH/NH_2 and OH/NO_2. The results indicate that the edge modification of the OH/SO_2 that causes a asymmetric energy band improves the electron transport of the device, suggesting a method to design graphene rectifier with good performance.

1. Introduction

In recent years, graphene has attracted more attention experimentally and theoretically since it was synthesized [1,2]. Many graphene nanomaterials have been prepared, such as graphene nanoribbons (GNRs) [3,4], double-layer graphite structures [5,6], quantum junctions [7,8]. According to the different boundary structures, GNRs are mainly divided into zigzag-shaped graphene nanoribbons (ZGNRs) and armchair-shaped graphene nanoribbons (AGNRs). GNRs with different edge configurations exhibit different electrical properties, and have been widely used in the fields of transistors [9], sensor [10] and optoelectronic devices [11] because of flexible and adjustable bandgap [12,13]. The functional molecular devices based on GNRs will play a significant role in the design of molecular electronics in the future.

Since rectifier device with donor-bridge-acceptor-type organic molecules was proposed [14], molecular rectifier has been investigated extensively. Recently, a pretty rectifying behavior (the maximum rectification ratios can reach the order of 10^5) and a perfect (100%) spin filtering effect have been found in H2−5ZGNR−H with asymmetry-doped ZGNR electrodes [15]. The transport properties of ZGNR heterojunctions can be modulated by the different edge hydrogenations, and rectification effect also can be observed [16]. A new planar all-Graphene DB-RTD have been proposed, which reverse rectification ratio can exceed 5×10^4 [17]. The gas adsorption [18,19], defecting [20] and chemical doping [21,22] are the common methods to lead to a rectification. GNRs may be a breakthrough in the preparation of high performance rectifiers. Thus, it is important to study the transport properties of GNRs-based molecular rectifier.

In this work, based on density-functional theory (DFT) and nonequilibrium Green's function (NEGF), we investigate the electronic transport properties of zigzag-shaped graphene nanoribbons (ZGNRs) devices which have been modified by OH/NH_2, OH/NO_2 and OH/SO_2. One can see that the currents of A and B device show symmetry with small rectification effect and negative differential resistance (NDR) effect is observed. However, the (reverse) rectification ratio of device with edge modification of OH/SO_2 also are extremely small except at 0.2 V and 0.6 V where maximum rectification ratios is 2076.33 at 0.2 V, and maximum reverse rectification ratios is 1937.33 at 0.6 V. The functional groups modification affects the electronic transport property of the 12-ZGNRs.

2. Model and method

We design the molecular device based on 12-ZGNR to study the effect of different functional groups (OH/NH_2, OH/NO_2, OH/SO_2) on electronic transport of device by DFT and NEGF formalism as implemented in Atomistix ToolKit (ATK) [23,24]. In Fig. 1, the device is divided into left electrode (12-ZGNR), central scattering regions (12-ZGNR and 8-ZGNR) and right electrode (12-ZGNR), where the number represents the width of the nanoribbon. The edge of designed device is

* Corresponding author.
E-mail address: baoanbian@jiangnan.edu.cn (B. Bian).

http://dx.doi.org/10.1016/j.physe.2017.09.002
Received 16 February 2017; Received in revised form 15 June 2017; Accepted 5 September 2017
Available online 08 September 2017
1386-9477/

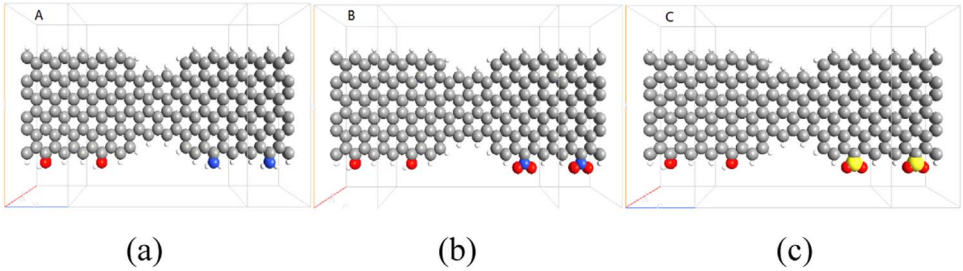

Fig. 1. The designed ZGNRs devices. The red, blue, yellow, white and gray spheres represent oxygen, nitrogen, sulfur, hydrogen and carbon atoms, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

modified by OH/NH_2 (Fig. 1(a)), OH/NO_2 (Fig. 1(b)) and OH/SO_2 (Fig. 1(c)) that are donated as A, B, C. In the present calculations, the Perdew-Zunger local-density approximation (LDA.PZ) [25] is used to describe the electron exchange correlation potential. All atoms adopt a double-zeta with polarization (DZP) basis set. The k-point grid is set to 3 × 3 × 300 and the mesh cutoff is adjusted to 150 Ry in order to achieve a balance between calculation efficiency and accuracy. Self-consistent calculations are performed with an iteration control parameter tolerance about 0.0001.

The current of device is calculated by Landauer–Bütiker formula [26]:

$$I(V_b) = \frac{2e}{h}\int_{\mu_l(V_b)}^{\mu_r(V_b)} T(E, V_b)dE$$

where μ_l and μ_r are the electrochemical potentials of the left and right electrodes, and $\mu_l - \mu_r = eV_b$. The electron transport coefficient can be obtained by

$$T(E, V_b) = Tr[\Gamma_l G^R \Gamma_r G^A]$$

where $G^{R/A}$ is retarded (delayed) Green's function. $\Gamma_{l/R}$ is the contact broadening functions associated with the left (right) electrode.

3. Results and discussion

Fig. 2(a) is the calculated current-voltage (I-V) curves for the three devices. It is clear that the I-V characteristics for devices A and B exhibit a similarity in the bias region of [– 1.2 V, 0.4 V], but the current of device B is larger than device A in the bias region of [0.5 V, 1.2 V]. The current of device C is smaller than devices A and B at whole bias. For the device A, the current decreases from 0.4V to 0.6 V, showing a negative differential resistance (NDR) effect, and the NDR effect in the region of bias from – 0.3 V to – 0.6 V and – 1 V to – 1.1 V is observed. The devices B and C also show the NDR effect. We calculate the rectification ratio (R(V) = I(V)/I(-V)) to describe the asymmetry of I–V curve in Fig. 2(b). A reverse rectification ratio is defined as RR(V) = I(V)/I(-V) in the inset of Fig. 2(b). It can be clearly observed that the rectification ratio of devices A and B are very small, and their maximum rectification ratios are 2.27 and 10.49 respectively. The (reverse) rectification ratio of device A is also extremely small except at 0.2 V and 0.6 V. For device C, maximum rectification ratios is 2076.33 at 0.2 V, and maximum reverse rectification ratios is 1937.33 at 0.6 V.

The electronic structure of a molecular device plays a significant role in explaining the transport properties [27]. In order to investigate the effect of functional groups modification on rectifying phenomenon, the transmission spectra and the energy band structures of the related electrodes for these devices at different bias are plotted in Fig. 3. In the calculations, the Fermi level is set to 0. One can see that the energy band structure of electrode changes with the different functional groups modification. The left electrode in three models at 0.6 V(– 0.6 V) has same band structures because they have same left electrode. However, the band structure of the right electrode varies with the different functional groups. The energy band of the electrode comes to shift with changing bias. Compared with Fig. 3(a) (Fig. 3(c), Fig. 3(e), Fig. 3(g)), the energy bands of the left electrode in Fig. 3(b) (Fig. 3(d), Fig. 3(f), Fig. 3(h)) move upwards, while the opposite motion can be observed for the energy bands of the right electrode. It is known that the coupling between the band structure of left and right electrodes cause a transmission peak [28,29]. For devices A and B, at the bias of ± 0.6 V, the band structure of the left electrode matches the right electrode, accounting for appearance of transmission peak in the bias window. Furthermore, the integral area of the transmission spectrum of Fig. 3(a) (Fig. 3(c)) is slightly larger than Fig. 3(b) (Fig. 3(d)) in the bias window, which causes a small difference of current between 0.6 V and – 0.6 V. Therefore, the modified edges by OH/NH_2 and OH/NO_2 result in a very poor rectification in devices A and B. For device C, as shown in Fig. 3(e) and (f) (Fig. 3(g) and (h)), there are not the transmission peaks at the bias of 0.6 V(– 0.2 V) in the bias window. There is a transmission peak in the bias window at the bias of – 0.6 V(0.2 V), displaying the rectification phenomenon. Therefore, the asymmetric band structure contributes to the rectifying behavior [28].

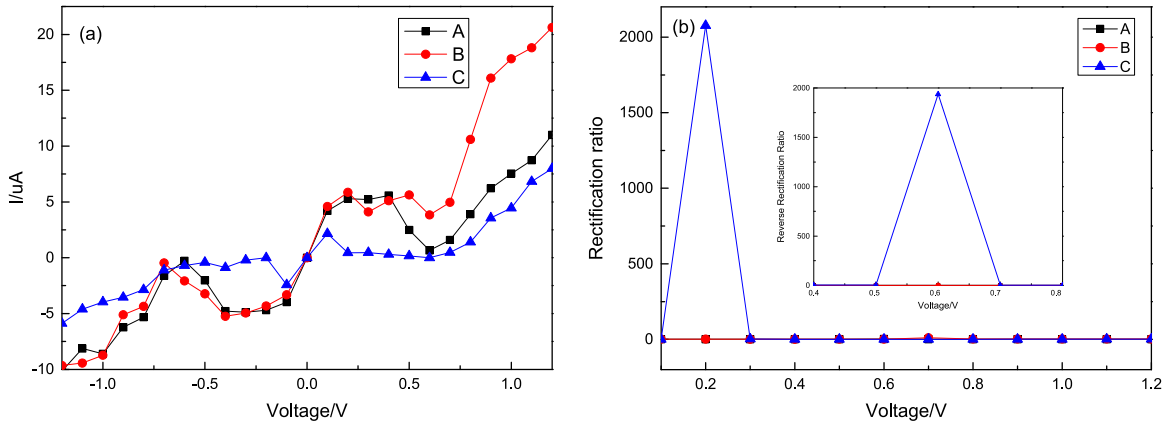

Fig. 2. (a) The current–voltage curves for device A, B and C. (b) the rectification ratio R(V) and the reverse rectification ratio RR(V) for these devices.