Organic Electronics 48 (2017) 1–6

Contents lists available at ScienceDirect

Organic Electronics

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

Tuning the I–V characteristic of a cruciform diamine molecular device by connected position and B/N doping

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ARTICLE INFO

Article history:
Received 1 March 2017
Received in revised form
4 May 2017
Accepted 14 May 2017
Available online 18 May 2017

Keywords:
Molecular device
Transport properties
B/N doping
Negative differential resistance

ABSTRACT

By performing first-principle quantum transport calculations, we investigate the effects of connected position and B/N doping on the transport properties of a single cruciform diamine molecule connected to zigzag graphene nanoribbon leads. The negative differential resistance behaviors are found in I–V characteristics of the undoped molecular device. The peak-to-valley current ratio can be modulated obviously by changing the connected position. Then, we find the B/N doped effects are sensitive to doping site in the connected region. The replacement of B/N atom on R1 (carbon atom in connected region close to the zigzag graphene nanoribbon) seldom affects the transmission spectrum around Fermi level. But, the replacement of B/N atom on R2 (carbon atom in connected region close to the molecule) can raise the transmission coefficient around Fermi level markedly leading to the large growth of the current at the low biases. In addition, the replacement of N atom on R2 can induce a negative differential resistance behavior in I–V curve at low bias region.

1. Introduction

The discovery of atom-thin sheets of carbon known as graphene leads to the scale of the functional devices decreasing to two-dimension [1]. Because of its unique physical properties, such as high carrier mobility [2], long spin relaxation times [3], and room temperature quantum Hall effect [4], graphene is regarded as a novel and very prospective material for the future generation of electronic devices, photoelectric devices and spintronics devices [5–8]. Moreover, one-dimensional graphene nanoribbons (GNRs) are adopted as the electrode in designing of the molecular devices as a result to further reduce the size of the functional devices. As compared with the metal, the edge styles (zigzag or armchair) were found to play a pivotal role in the observed charge-transport behavior of these GNRs [9,10]. So far, various molecular devices based GNR electrode have been fabricated in experiment or designed by theoretical methods. The oscillatory conductance was also found in atomic carbon wire-graphene junctions for even-odd number of carbon atoms [11,12]. Switching, rectifying and negative differential resistance (NDR) are also found in the molecule-graphene junctions [13–17]. In addition, excellent spin-filter and spin valve had been found in several molecules between two GNRs [18–21].

In order to modulate the transport properties of the molecular devices based GNR electrode, a lot of physical and chemical methods have been proposed [22–24]. Among them, the B/N doping is generally considered as a simple and effective method because their atomic size and the electronic structure are similar to the carbon atom. Electronic structures and transport properties of armchair graphene nanoribbon (AGNR) and zigzag graphene nanoribbon (ZGNR) all can be modulated significantly by ordered doping of B or N atoms [25,26]. The hybridization of h-BN nanoribbon can make the ZGNR perform the NDR or rectifying behaviors [27,28]. The periodical B/N doping in semi-infinite graphene electrodes can achieve an excellent rectification in a molecule-graphene junction [29]. It is well known, the nature of the molecule-electrode interface plays an important role in the charge transport of the molecular devices [30]. Therefore, in this paper, we investigate the effect of connecting position on the transport

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http://dx.doi.org/10.1016/j.orgel.2017.05.030
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properties of a single cruciform diamine molecule connected to zigzag graphene nanoribbon leads. Moreover, the effect of B/N doping in the connected region on the transport properties of the molecular junction is also studied. The calculated results should be valuable for deeply understanding the relationship between the contact interface and the charge transport mechanism of the molecular devices.

2. Model and method

The molecular device is shown in Fig. 1. A single cruciform diamine molecule (CDM) covalently bridges two ZGNR electrodes. All edge carbon atoms of ZGNR are saturated with hydrogen atoms. The device is divided into three regions: left electrode, right electrode, and central scattering region. The central scattering region contains three units of ZGNR electrode on each side, thereby establishing the bonding between the molecules and the electrodes, the common Fermi level, and charge neutrality at equilibrium. R1 and R2 are two doping sites in the connected region between the ZGNR and the molecule. M1 and M2 are two types of the molecule connecting to the ZGNR. The CDM in M2 rotates 90° relative to M1. For simplicity, the B/N doping on R1 and R2 are named BR1, NR1, BR2 and NR2, respectively.

The geometric optimizations and the electron transport properties were calculated by using the first-principle software package Atomistix ToolKit (ATK), which is based on density-functional theory (DFT) in combination with the non-equilibrium Green's function (NEGF) [31,32]. The exchange-correlation potential is described by the local density approximation (LDA) and the wave function is expanded by the double-zeta plus polarization (DZP) basis for all atoms. The k-point sampling is 1, 1, and 100 in the x, y, and z directions, respectively, where the z is the periodic direction of nanoribbons. The real space grid techniques are used with the energy cut off of 150 Ry as a required cut off energy in numerical integrations and the solution of Poisson equation using fast Fourier transform (FFT). The geometries are optimized until all residual force on each atom is less than 0.05 eV Å^{-1}. The current $I(V_b)$ can be calculated by the Landauer formula: $I(V_b) = \frac{2e}{h}\int T(E,V_b)[f_L(E,V_b) - f_R(E,V_b)]dE$ [33,34]. Here, V_b is the bias voltage, $T(E,V_b)$ is the transmission coefficient, $f_L(E,V_b)$ and $f_R(E,V_b)$ are the Fermi-Dirac distribution functions of the left and right electrodes.

3. Results and discussion

In Fig. 2(a), we show the transmission spectra of M1 and M2 at the zero bias. From the figure, one can see two transmission peaks of M1 all locate in the positive energy region. The transmission peak close to the Fermi energy is broad but low. Another high and narrow transmission peak locates on 1.58 eV which is generated by the lowest unoccupied molecular orbital (LUMO). From the insert figure, one can see the molecular projected self-consistent Hamiltonian (MPSH) of this orbital mainly localizes on the central molecule which indicates it is a non-resonant tunnel. The MPSH is the self-consistent Hamiltonian of the isolated molecule in the presence of the electrode which can help us to understand the origin of the transport characteristics. That's why this transmission peak is narrow. When the molecule rotates 90° relative to M1, the transmission peak generated by LUMO of M2 is still narrow because the MPSH of this orbital localizes on the central molecule as before. But, it shifts to Fermi level and locates on 1.07 eV. As a result, the transmission coefficients around the Fermi energy are enhanced obviously. That means the connected position can affect the conductance of this molecular device. In order to prove it, we calculate the current-voltage (I–V) characteristics of M1 and M2 and show them in Fig. 2(b). From the figure, one can see the currents of M2 are indeed bigger than that of M1 before 1.4 V. The current of M1 reaches the peak value at 1.4 V and then decreases with bias voltage until 1.8 V. The current of M2 reaches the peak value at 1.2 V and then decreases with bias voltage until 1.8 V. Consequently, the I–V characteristics of GNR-CDM-GNR junction can present the NDR behaviors. Because M2 has the higher peak current and lower valley current, its peak-to-valley current ratio is

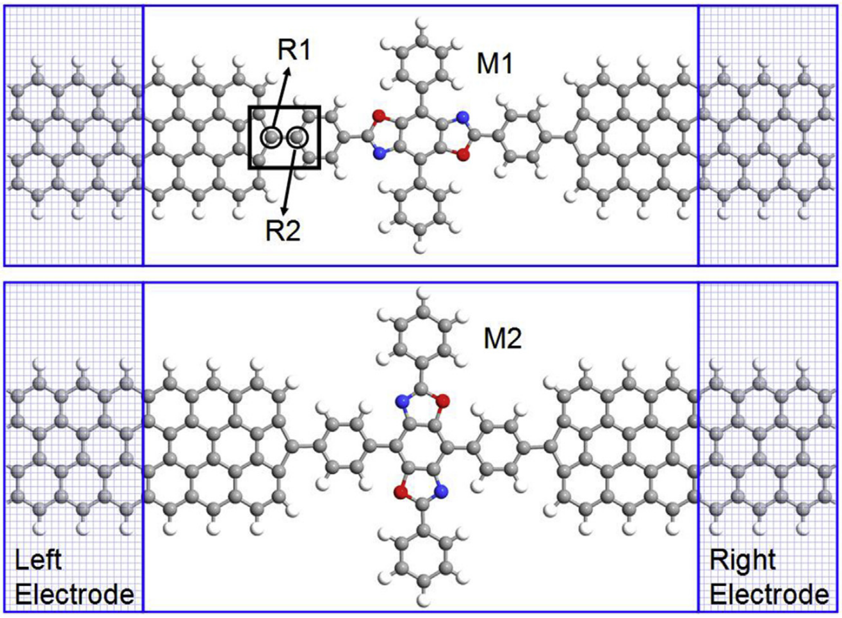

Fig. 1. Geometry Schematic illustration of the GNR-CDM-GNR junction. Black solid box indicates the connected region between the ZGNR and the molecule which includes six carbon atoms. R1 (carbon atom in connected region close to the ZGNR) and R2 (carbon atom in connected region close to the molecule) are two doping sites for B/N atoms. The red balls indicate oxygen atom and the blue balls indicate nitrogen atom, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)