Organic Electronics 15 (2014) 3674–3680

Contents lists available at ScienceDirect

Organic Electronics

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

Spin negative differential resistance and high spin filtering behavior realized by devices based on graphene nanoribbons and graphitic carbon nitrides

Xiangru Kong [a], Bin Cui [a], Wenkai Zhao [a], Jingfen Zhao [a], Dongmei Li [a], Desheng Liu [a,b,*]

[a] School of Physics, State Key Laboratory of Crystal Materials, Shandong University, Jinan 250100, People's Republic of China
[b] Department of Physics, Jining University, Qufu 273155, People's Republic of China

ARTICLE INFO

Article history:
Received 19 July 2014
Received in revised form 25 September 2014
Accepted 13 October 2014
Available online 28 October 2014

Keywords:
First-principles calculation
Graphene nanoribbons
Negative differential resistance
Spin filtering behavior

ABSTRACT

Using nonequilibrium Green's functions in combination with the density functional theory, we investigate the spin-dependent electronic transport properties of two nanostructure devices based on graphitic carbon nitrides bridging two zigzag graphene nanoribbons, i.e., center and edge bridged devices, respectively. It is found that the center bridged device behaves spin negative differential resistance properties in different bias ranges for the up and down spin current respectively. The edge bridged device presents obvious negative differential resistance only for the down spin current. Moreover, high spin-filtering efficiency over 80% is obtained in the edge bridged device in the bias range of 0–1.0 V. The magnetic properties of these devices suggest promising applications in spintronics and molecular electronics.

1. Introduction

Spintronics emerging from electronics in which the spin degree of freedom of electron is taken into account currently represents one of the most promising fields for future nanoelectronic applications [1–3]. There has been increasing interest in spintronic devices based on organic materials, especially on graphene [4,5] that was first discovered experimentally in 2004 and has aroused tremendous interest in the past decade [6–9]. As one-atom-thick planar material, graphene can be easily designed as functionalized nanodevices by cutting it into various shapes [10], changing its geometric configurations [11], chemical doping [12], introducing vacancy [13] and so on. Many interesting magnetic properties of graphene [14,15], such as rectification [16], spin filtering [17] and spin negative differential resistance (NDR) [18–20], have been reported. Graphene nanoribbons (GNRs) have been widely studied due to their characteristic properties of special edge. One of the most intriguing GNRs is obtained by cutting along the zigzag direction, i.e., zigzag-edged GNRs (ZGNRs). Previous investigations have shown that the electronic transport properties of ZGNRs depend on the two antiferromagnetically coupled edge states near the Fermi level [21]. Furthermore, this coupling could be tuned to be ferromagnetic by applying an experimentally accessible magnetic field [22,23]. This makes ZGNRs exhibit of great potential application in spin transporting nanodevice designing.

Meanwhile, graphitic carbon nitrides (g-C3N4) have recently attracted considerable attention because of its promising application in electronic devices [24,25]. The g-C3N4 can be synthesized by a variety of methods [26] and are regarded as the most stable allotrope of various nanostructure carbon nitrides in ambient conditions. The electronic structure of g-C3N4 differs significantly from

* Corresponding author at: School of Physics, State Key Laboratory of Crystal Materials, Shandong University, Jinan 250100, People's Republic of China. Tel.: +86 15376561777.
E-mail address: liuds@sdu.edu.cn (D. Liu).

http://dx.doi.org/10.1016/j.orgel.2014.10.016
1566-1199/

that of graphene. Spin-polarization and ferromagnetism behaviors have been reported in the modified s-triazine-based g-C3N4 [27]. On the other hand, the g-C3N4 can be combined to or embraced in graphene flakes [24,28–30], the compound of which can be regarded as graphene with regular nitrogen doping and vacancies. This opens the gate of constructing two probe system containing g-C3N4 on the basis of graphene.

In this paper, we propose two devices, M1 and M2 as shown in Fig. 1(a) and (b), based on graphitic carbon nitrides bridging two 4-ZGNRs electrodes. The graphitic carbon nitrides (C6N7H) labeled as M1B and M2B, respectively, can be considered as a periodic unit cut from the s-triazine-based g-C3N4. The dangling bond of carbon atom is terminated with hydrogen atom and nitrogen atoms leaving unhydrogenated. According to the bridged position, device M1 is referred to as the center bridged device while device M2 as the edge bridged device. The central scattering regions containing parts of the two electrodes form extended molecules to keep the potential continuous at the interfaces between the C6N7H and 4-ZGNR electrodes. The embraced parts of left (right) electrodes are specified by the label of A (C). The results, as will be shown below, indicate that both devices present spin NDR properties and the edge bridged device displays high spin-flittering phenomenon.

2. Computational method

The devices shown in Fig. 1 can be partitioned into three parts: the semi-infinite left electrode marked by green, the central scattering region, and the semi-infinite right electrode marked by yellow. In our calculations, we only consider the edge states under a ferromagnetic coupling for 4-ZGNRs electrodes. The geometrical optimizations and the electronic transport properties are calculated by the *ab initio* code package Atomistix ToolKit (ATK), which is based on the combination of density functional theory (DFT) with the non-equilibrium Green's function (NEGF) technique [31]. The single zeta polarization basis set is used for all atoms in our constructed devices. The cutoff energy is set to be 150 Ry and the mesh grid of the k space is $1 \times 1 \times 100$. The exchange–correlation potential takes the form of the Perdew–Zunger parametrization of the local spin density approximation (LSDA) which works well in previous works [17–20].

According to NEGF formulas, the spin-dependent currents through the scattering region are calculated by the Landauer-like formula [32]:

$$I_\sigma(V_b) = \frac{e}{\hbar}\int_{\mu_r(V_b)}^{\mu_l(V_b)} T_\sigma(E,V_b)[f_l(E,V_b) - f_r(E,V_b)]\,dE \qquad (1)$$

Here, $\sigma = \uparrow$ (spin up) and $\sigma = \downarrow$ (spin down), $T_\sigma(E,V_b)$ is the bias-dependent and spin-dependent transmission coefficient, $f_{l(r)}(E,V_b)$ is the Fermi–Dirac distribution function of the left (right) electrode. $\mu_{l(r)}(E,V_b)$ is the electrochemical potentials corresponds to the left or right electrode. Considering the fact that the Fermi level is set to be zero, the region of the energy integral window $[\mu_l(E,V_b), \mu_r(E,V_b)]$ can be written as $[-V_b/2, V_b/2]$.

3. Results and discussions

We show our calculated currents of the two probe systems in Fig. 1(c) and (d) as a function of the bias varying from 0 V to 2.0 V. Fig. 1(c) displays that NDR behavior occurs in different bias ranges for different spin channel in device M1. In the case of the up spin current, the NDR

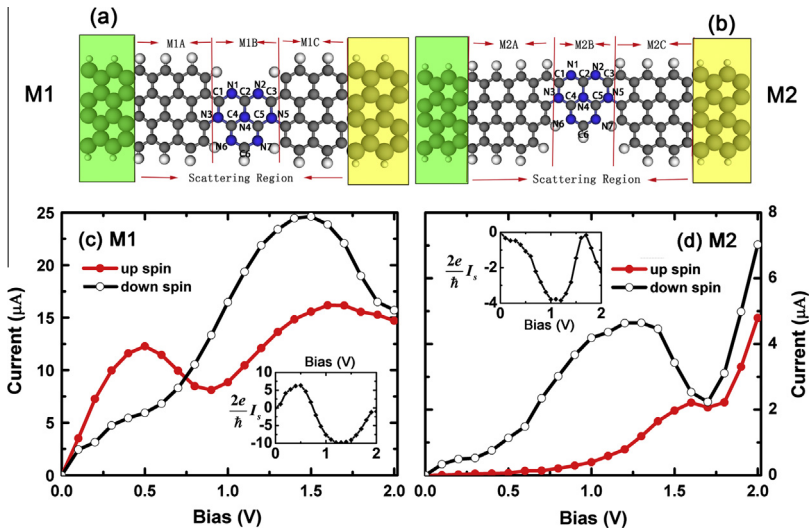

Fig. 1. (a) and (b) Correspond to the center bridged device M1 and the edge bridged device M2 which are based on graphitic carbon nitrides bridging two 4-ZGNRs electrodes. The semi-infinite left electrode is marked by green, the central scattering region is divided into three parts labeled as M1A (M2A), M1B (M2B) and M1C (M2C) respectively, and the semi-infinite right electrode is marked by yellow. (c) and (d) Correspond to the calculated spin resolved current for device M1 and M2. The red solid circle line corresponds to the up spin current and the black hollow circle line corresponds to the down spin current. The insets in (c) and (d) correspond to the spin current for device M1 and M2, respectively. C1, C2, . . .,C6 and N1, N2, . . ., N7 represent carbon atoms and nitrogen atoms in M1B/M2B, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)