Organic Electronics 15 (2014) 1012–1017

Contents lists available at ScienceDirect

Organic Electronics

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

Improving spin-filtering efficiency in graphene and boron nitride nanoribbon heterostructure decorated with chromium-ligand

Jing Zeng [a,*], Liezun Chen [a], Ke-Qiu Chen [b]

[a] Department of Physics and Electronic Information Science, Hengyang Normal University, Hengyang 421002, China
[b] Department of Applied Physics, Hunan University and Key Lab for Micro-Nano Physics and Technology of Hunan Province, Changsha 410082, China

ARTICLE INFO

Article history:
Received 19 December 2013
Received in revised form 26 January 2014
Accepted 12 February 2014
Available online 26 February 2014

Keywords:
Spin transport in nanoscale materials and structures
Spin-filtering effect
Molecular magnets

ABSTRACT

By applying nonequilibrium Green's functions in combination with density-function theory, we investigate the spin-dependent transport properties of graphene and boron nitride nanoribbon heterostructure decorated with chromium-ligand. In the heterostructure, the graphene and boron nitride nanoribbon are connected in a interlaced way, and the chromium-ligand are decorated above the surface of the graphene nanoribbon. When one boron nitride nanoribbon fragment is embedded in the graphene nanoribbon, the maximum spin-filtering efficiency at finite bias is only about 65%. However, almost 100% spin-filtering efficiency can be observed at low bias when one more BNNR fragment is introduced into the system. Especially, the high spin-filtering efficiency is independent of the magnetic configuration of the device. Our work provides a new thinking to achieve the high-performance spin filter.

1. Introduction

Recently, the molecular spin filter has become an interesting topic due to its potential application in next-generation circuits [1–9]. With the advancement of experimental technique and theoretical method, various kinds of nanomaterial, such as metal-phthalocyanine [1,2], 6, 6, 12-graphyne nanoribbons [3], graphene nanoribbon [4,5], carbon atomic chains [6], porphyrin [7,8], and Mn-doped thiolated Au_{25} nanoclusters [9], have been proved to possess tremendous potential for designing the spin filter in the future. Very likely origins of the spin filtering properties in these nanomaterial, such as the symmetry matching of wave functions of spin subbands [4], the difference of orbitals numbers in different spin states [5], the distribution difference of electronic states for both spin polarizations [8], localized magnetic moment protected by ligand [9] were also proposed.

Recently, graphene has been identified as a perfect nanomaterial for constructing the molecular device [10–14]. To further broaden its application, many feasible ways have also been adopted to tune its electronic properties, such as hybridization [15–19], surface adsorption [20], chemical modification [21], and external strain [22]. In particular, the hybridization about graphene and boron nitride sheet, has attracted much interest among researchers. Experimentally, the graphene-boron nitride hybridization system has been successfully fabricated [15,16], opening up the door for its potential application in the future. Meanwhile, many theoretical studies show that once the electrically conductive graphene and insulating boron nitride sheet is connected with each other, the hybridization system will present interesting electronic and magnetic properties [17–19]. However, there are only a few theoretical studies on the transport properties of the

* Corresponding author. Tel.: +86 15211898336.
E-mail address: hyzengj@126.com (J. Zeng).

http://dx.doi.org/10.1016/j.orgel.2014.02.010
1566-1199/

graphene-boron nitride hybridization system [23]. As we know, the electronic property of nanomaterial cannot represent the entire transport characteristics of the system [24]. Therefore, in the present paper, a graphene and boron nitride nanoribbon-based electronic device is constructed to study the corresponding transport properties under the finite bias. Our results show that the hybridization system can present interesting spin-filtering effect. Especially, the maximum spin-filtering efficiency of the system at finite bias can be increased from about 65% to almost 100% by adding the BNNR fragment in the system, indicating that the system possesses the potential value for designing as a high-performance spin filter.

2. Model and formalism

The hybridization system we investigate is shown in Fig. 1. The system is constructed with zigzag graphene nanoribbon (ZGNR) and zigzag boron nitride nanoribbon (ZBNNR). It is noted that the ZGNR and the ZBNNR are connected in a interlaced way. To facilitate discussion, the devices in Fig. 1(a) and (c) are named as M1 and M2, respectively. In the two devices, both left and right electrodes are described by a supercell with two repeated ZGNR unit cells along transport direction. It is known that the electronic states of the ZGNR can be non-magnetic, antiferromagnetic, or ferromagnetic states, depending upon the external means [4]. In the present work, the ZGNR electrodes are considered as the spin-unpolarized state [24]. Moreover, For M1 (M2), the number of unit cells for ZGNR and ZBNNR in the central scattering region are 12 (16) and 4 (8), respectively. We can see from Fig. 1(a) that one ZBNNR fragment is embedded in the ZGNR and thus the ZGNR in the central region are separated into two regions (namely, G1 and G2). It is well known that the ZBNNR has a large energy gap [21], thus it acts as a tunneling barrier in the central region. Meanwhile, two metal-ligands (metal-C_6H_6) are adsorbed on the hollow site of the G1 and G2 regions. As previous report shows that Cr–C_6H_6 group can be stably adsorbed on the surface of the graphene, the Cr–C_6H_6 group is chosen in our work [25]. In the device, the distance between two Cr atoms is about 19.7 Å, so their spin directions can be tuned independently [7,8]. This means that the change of magnetic configurations can be readily realized by applying the external magnetic field. As a result, the device can be set as ferromagnetic (↑↑) and antiferromagnetic (↑↓) configurations. For convenience, these two magnetic configurations (↑↑ and ↑↓) are called as $M1_{\uparrow\uparrow}$ and $M1_{\uparrow\downarrow}$, respectively. In order to investigate the tunneling barrier dependence of transport properties in the hybridization system, one more BNNR fragment is increased, which corresponds to M2 (see Fig. 1(c)). Clearly, for the M2, two ZBNNR fragments are embedded in the ZGNR. As a result, there are three ZGNR regions in the central region (namely, G1, G2 and G3). Each region is adsorbed one Cr–C_6H_6 group. Therefore, in contrast to the M1, there are one ferromagnetic configuration (↑↑↑) and two antiferromagnetic configurations (↑↓↑ and ↑↓↓). Similar to the M1, these three magnetic configurations (↑↑↑, ↑↓↑ and ↑↓↓) are called $M2_{\uparrow\uparrow\uparrow}$, $M2_{\uparrow\downarrow\uparrow}$ and $M2_{\uparrow\downarrow\downarrow}$, respectively. In the present work, we investigate the transport properties of the $M1_{\uparrow\uparrow}$, $M1_{\uparrow\downarrow}$, $M2_{\uparrow\uparrow\uparrow}$, $M2_{\uparrow\downarrow\uparrow}$ and $M2_{\uparrow\downarrow\downarrow}$, and thus assess the effect of tunneling barrier on transport properties in the hybridization system. The quantum transport calculations have been carried out by using the first-principles method based on

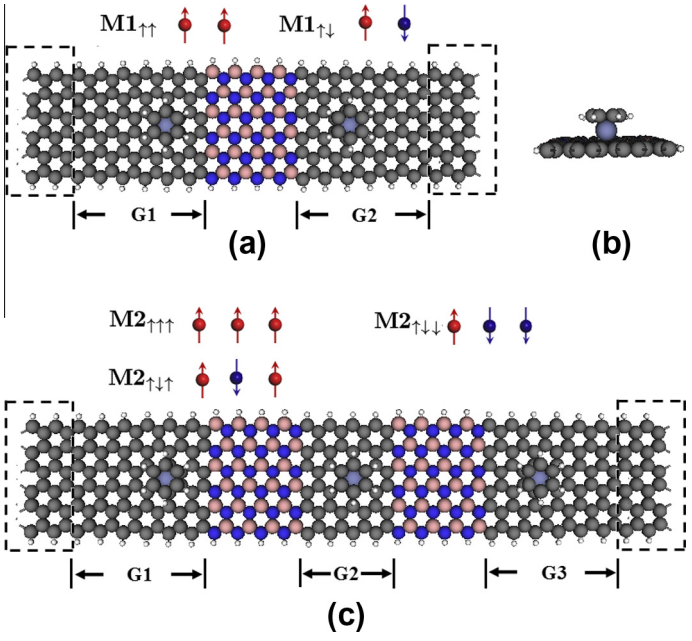

Fig. 1. Schematic view of the hybridization system constructed with zigzag graphene nanoribbon and zigzag boron nitride nanoribbon. (a) The top view of the M1. If the spin directions of the two Cr atoms are set in parallel (antiparallel), the device are called as $M1_{\uparrow\uparrow}$ ($M1_{\uparrow\downarrow}$). (b) The side view of the M1. (c) The top view of the M2. If the spin directions of the three Cr atoms are set in parallel (antiparallel), the device are called as $M2_{\uparrow\uparrow\uparrow}$ ($M2_{\uparrow\downarrow\uparrow}$ and $M2_{\uparrow\downarrow\downarrow}$).