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Coupling site controlled spin transport through the graphene nanoribbon junction: A first principles investigation

Jiming Zheng [a,*], Xiaoqing Deng [b], Jianwei Zhao [c], Ping Guo [d], Chongfeng Guo [a], Zhaoyu Ren [a], Jintao Bai [a]

[a] *Institute of Photonics & Photo-Technology, National Key Laboratory of Photoelectric Technology and Functional Materials (Culture Base), National Photoelectric Technology and Functional Materials & Application of Science and Technology International Cooperation Base, Northwest University, Xi'an 710069, People's Republic of China*

[b] *School of Physics and Electronic Science, Changsha University of Science and Technology, Changsha 410004, People's Republic of China*

[c] *School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210008, People's Republic of China*

[d] *Department of Physics, Northwest University, Xi'an 710069, People's Republic of China*

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ABSTRACT

A new type of nano-junctions based on Zigzag graphene nanoribbons (ZGNRs) has been proposed and investigated by first-principles calculations. The results show that large spin polarization of currents would be achieved when the junctions adopted the configuration that two ZGNR leads coupled each other along one edge. By virtue of spatial separation of the two spin edge states, only one spin channel is opened in those junctions at certain energy range, and spin polarized currents will be produced under a low bias. No more efforts are required to change ZGNR from the antiferromagnetic (AFM) ground states to the ferromagnetic (FM) states. Specially, this feature is stable, by changing the width of ZGNRs, modifying the edge morphology, and varying dihedral angle between two ZGNRs, spin polarization of currents are still observed. Our findings indicate that this approach is simple and efficient for spintronics design.

1. Introduction

Graphene based spintronics are promising candidates for next generation of information devices. The pristine graphene present a spin degenerated Dirac-like electron dispersion at the *K* points of the Brillouin zone. When it is cut into one-dimensional ribbons with Zigzag edges, spin polarized local edge states occur. Exploiting those edge states to enhance the performance of ZGNRs devices is a hot topic in the research community. Son et al. first show that transverse electrical fields can make ZGNRs half-metals [1]. Soon after, chemical decoration and doping are proved to be an alternative way to convert ZGNR half-metal [2,3]. Following those ideas, many ZGNR junctions have been designed to perform as spin-filter, spin-valve and spin caloritronics devices. Generally, four points are the keys for device design: edge decoration [4–6], central scattering region design [7–10], external field layout and band symmetry matching [11–15].

For example, Jun Kang et al. proposed an asymmetrically hydrogenated ZGNR, whose spin up valence states are below Fermi level (EF) while the spin down conduction states are just above EF. Through p-type or n-type doping, this ZGNR can give rise to 100% spin filtering effect [4]. Zeng et al. applied carbon atom chain as central scattering region and find the simultaneous occurrence of spin-filter and spin-valve in a single device [8]. Sahin and Senger designed a junction whose central scattering region was consisted of a graphene flake and some magnetic adatoms, that could also induce spin polarized current [10]. Zeng et al. studied the effect of magnetic layout of two leads which can be set to parallel [1,1], antiparallel [−1,1] and [1,0] (one electrode is magnetized while the other is nonmagnetic), and significant influence on spin transport properties of the junctions are observed [11]. A similar result was reported by Zeng [12] and combined, another important factor to spin polarized current – band symmetry was studied in this paper.

All those work has a common goal: managing to induce the spin polarized bands of ZGNRs. Because the ground state of ZGNRs is antiferromagnetic (AFM) with zero total magnetic moment, hence no halfmetallicity occurs unless doping or inducing external fields, topological line defect, and strain into ZGNRs [1,16–29]. It is worth to note that spin-polarized electronic states localized along the two edges of ZGNRs are individually ferromagnetically (FM) ordered but antiferromagnetically coupled to each other through the graphene backbone [25], and that the current mostly flows along the edge of GNR under low bias [30]. Based on these distinguishing features, we proposed that spin up and spin down currents are localized along edges and separated from each other. If we keep one edge intact and cut off the other one, then only one kind of spin

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* Corresponding author.

E-mail addresses: zjm@nwu.edu.cn (J. Zheng), xq_deng@163.com (X. Deng).

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currents would be preserved. So, we design a new type of junction using spatially separated ZGNRs' edge states in this paper, which was proved to be simple and efficient in obtaining spin polarized current.

2. Model and computational details

Our models are shown in Fig. 1. The junctions are all composed by ZGNRs. We align one edge of each ZGNR leads (two units cell of ZGNR along the transport direction are used as the left/right leads) and keep the other two edges on the both sides of this line, naming it A1-junction, while, for comparison, perfect ZGNR junction are named A2-junction. The systems are described by density functional theory (DFT) with the norm-conserving pseudopotential and the quantum spin transmission is evaluated by the nonequilibrium Green's function (NEGF) technique, using the software package QUANTUMWISE [31–33].The wave functions are expanded on a numerical basis set of single-ζplus polarization (SZP) for all atoms. The local spin density approximation (LSDA) with the Perdew–Zunger parametrization of the correlation energy is used for the exchange–correlation functional. The mesh cutoff is 150 Ry which is the default value.

3. Results and discussion

Fig. 2 gives the spin polarized current–voltage (*I*–*V*) characteristics of each model. It is apparently different between A1-junction's *IV*-curve and that of A2-junction, as shown in Fig. 2a and b. Large spin polarization of current in A1-junction under 0.6 V bias is observed, as shown in Fig. 2a. In contrast to A1-junction, no spin polarization of current in A2-junction occurs in Fig. 2b. The spin filter efficiency (SFE) of A1-junciotn under a finite bias voltage, defined by SFE = $(I_{\mathrm{up}}-I_{\mathrm{down}})/(I_{\mathrm{up}}+I_{\mathrm{down}}) \times 100\%$, is shown in Fig. 2c. We find that when bias change from -0.7 V to 0.7 V, large SFE are achieved, most of them larger than 90%, especially at 0.5 V–0.6 V, SFE are larger than 95%. When we further increases the bias, SFE begin to decrease. In spite of large SFE in bias range from -0.3 V to 0.3 V, the currents are too low (in order of $\sim 10^{-11}$A as shown in Fig. 2d) to be detected. So, 0.4 V–0.6 V would be a proper bias range for the further experimental studies. The sharp falling of SFE at 0.3 V bias is resulted in the relatively quicker increase of down-spin current (from 3.06e-13 A at 0.2V bias to 1.18e-11 A at 0.3 V) than that of up-spin current (from 9.01e-12 A at 0.2 V bias to 2.39e-11 A at 0.3 V) in the bias range from 0.1 V to 0.3 V, seeing in the Fig. 2d where logarithmic coordinate is used to show the trend clearly.

Next, we explain the reason why spin polarization of current is so sensitive to the coupling site between ZGNRs. We start from the analysis of the electronic band structure and transmission spectrum of the junctions under equilibrium state. Band structure of the ZGNR (with 8 zigzag chains across the ribbon section) is shown in the left panel of the Fig. 3a, and the transmission spectrum of A1-junction is in the right panel. Two peaks in different spin channels in the transmission spectrum are observed just at the both sides of the E_F. Correspondingly, both of the valence band (VB) and conduction band (CB) of ZGNR have a flat portion here, which will give rise to large and localized density of states (DOS) inducing large transmission peaks in this energy range. But, note that the transmission spectrums are spin polarized, while ZGNRs are at AFM state and show spin degenerated band structure.

We then turn to calculate the Bloch states of ZGNR at some K points of the VB and CB. The Bloch states at the flat portion of the VB and CB locate along the edge of ZGNRs. For the same band, the up-spin edge states locate along one edge and down-spin counterparts along the other. While for the same edge, it is occupied by the VB edge states and the CB edge states of different spin alternatively. When the Bloch states are at the K points out of the flat portion they will soon spread across the section of the ribbon (The similar results have already been reported by others [16] and then no figures are shown here). This feature is important. It will give rise to different coupling between ZGNRs in different spin channels if we change the edge coupling between two ZGNRs.

For A1-junction, there is only one aligned edge between the two ZGNRs and the atoms of this edge all have the same spin orientation (We also set the aligned edge of the two ZGNRs to the opposite spin, but find that it has higher energy, about 100 meV, than the junction with the same spin in the aligned edge). Beneath the E_F, coupled VB states between the two ZGNRs leads are just those edge states. While the other edge states in spin down channel at the same energy are localized along the two separated edges, and there are no coupling between them, as shown in the LDOS in Fig. 3b. This is the reason why only spin up channel is opened below E_F. Above the E_F, things are a little different. Transmission peaks of both spin channels can be observed. A large spin down peak is above the flat portion of the CB. While a little spin up peak just corresponds to that portion of the CB. This peak means that transmission between two lead in spin up channel is still probably even two spin up CB edge states are separated as shown in middle panel of Fig. 3b. And although the spin down CB edge states are now along the aligned edge, the large transmission peak still occurs at higher energy implying that strong coupling between spin down CB states is postponed to the energy range that the spin down CB states have spread across the section of ZGNRs.

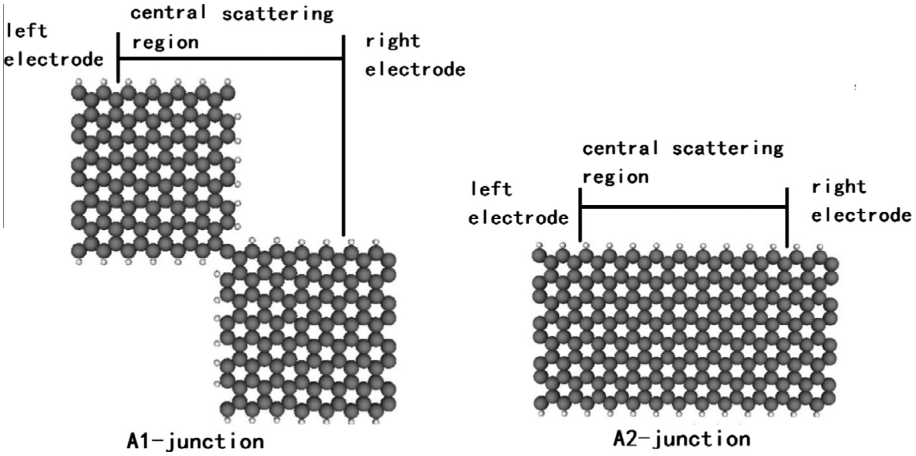

Fig. 1. The schematic illustration of the ZGNRs junctions, where two units cell of ZGNR along the transport direction are used as the left/right leads.