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Spin filter effect in the zigzag graphene nanoribbons

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Spin filter effect in the zigzag graphene nanoribbons

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Abstract. The spin-related transport properties of graphene nanoribbons with zigzag edges which are partially coupled to Au linear-chain electrodes have been investigated by using non-equilibrium Green's function in combination with the density-functional theory. The results show that the partial contact with the electrodes will break the spin degeneracy, leading to the completely spin-polarized transport. Meanwhile, the spin-related properties are obviously dependent on the electrodes contact positions. For the boron doped graphene nanoribbons, the spin polarized effect is enhanced.

1. Introduction

Recently, the electronic transport properties of the graphene nanoribbons (GNRs) have been paid widely concerned [1-4]. In particular, graphene nanoribbons having R zigzag rows (R-ZGNR) have been most intensely studied due to the characteristics of the spin-polarized ground state [5,6]. And the spin is degenerate because the total charge difference between up spin and down spin electrons is zero. Therefore, in order to obtain spin-polarized current, we must break the degeneracy. Some feasible approaches have been proposed to change the transport properties of the ZGNR, such as external electrical field [7], defect [8], doping [9,10], molecule adsorption [11], and graphene nano-junction [12,13]. These approaches provide plenty of opportunities to enlarge the applications in spin-based electronic devices, because of completely spin-polarized current can be obtained. Among most of these possibilities, the ZGNR as the scattering region is completely linked to two electrodes. However, it is impossible to get spin-polarized transport for perfect ZGNR because of the geometrical symmetry between the contact electrodes and the scattering region.

In this letter, the investigated scattering region contacts to the electrodes partially, and we mainly study the effect of the electrode contact position and impurity on the spin-polarized transport. The partial contact with the electrodes can cause the spatial separation of spin states, which will break the spin degeneracy, leading to the spin-polarized transport. Especially, full spin polarization (100%) can be obtained at the Fermi level.

2. Computational method and model

In our system, the structure model is pristine ZGNR which is a perfect 4-ZGNR being cut four carbons at the edge [Fig.1 (a)]. According to convention labeling spin states, the down-spin (↓) are situated at the upper edge, and the up-spin (↑) are situated at the lower edge. So as to realize spin-polarized transmission, we design a two-probe model, the pristine ZGNR is partially contacted with linear Au atomic chains, which has been used by several groups for a variety of applications [14].

The $T(E)$ can be decomposed into the spin-dependent nonmixing eigenchannels $T_\sigma(E)$,

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$$T(E) = \sum_{\sigma} T_{\sigma}(E), \tag{1}$$

For each spin state σ the $T_{\sigma}(E)$ is expressed as

$$T_{\sigma}(E) = Tr\left[\Gamma_L G^r \Gamma_R G^a\right]_{\sigma}, \tag{2}$$

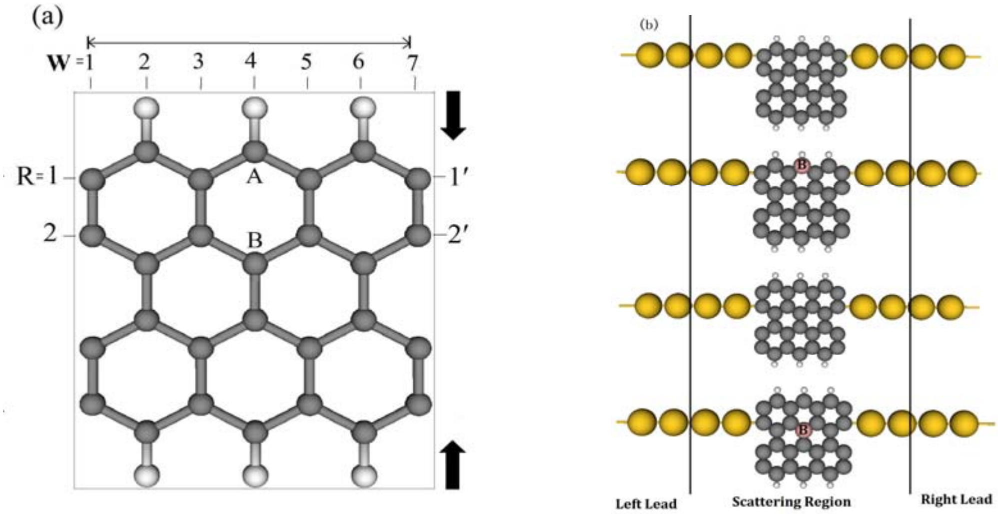

Figure 1. (a) A model for pristine ZGNR. *R* represents the number of zigzag chains and *W* is the width of ZGNR. Possible impurity sites are labeled as *A* and *B*. Left and right leads are linked to the ZGNR at the 1, 2 and 1, 2 respectively. (b) The structure model. Electrodes are attached to the pristine ZGNR and the boron doped pristine ZGNR at the 1-1, and at the 2-2 respectively.

3. Results and discussion

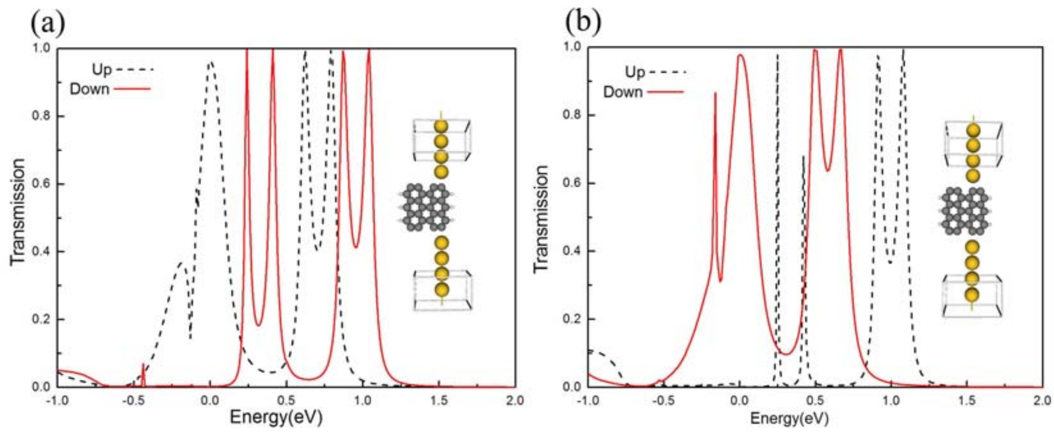

Figure 2. (Color online) Spin-dependent transmission spectrums of the pristine ZGNR. The insets show the contact geometries of electrodes (a) 1-1 site, (b) 2-2 site.

Fig. 2 describes the device of the pristine ZGNR with linear Au atomic chains electrodes contacted to one of the zigzag rows and the corresponding equilibrium transmission spectra. Due to the structural symmetry, it is study that the leads are linked to the 1-1 and 2-2 positions. Our calculations show that the effect of the electrodes contact location on the transmission spectrum is very dramatic, changing the transport behavior of the up-spin and down-spin electrons. When the leads link to the 1-1 position, the up-spin channel is conducted, but the down-spin channel is suppressed completely. Interestingly, with the leads making contact to the 2-2 site, it is just the opposite case compared to the 1-1 site, the up-spin channel is suppressed and the other is conducted.

From the research above, we can see that, with varying the electrodes contact positions from 1-1 site to 2-2 site, the up-spin channel (the black dashed line) transforms from 'conducted' state to 'suppressed' state, while the down-spin channel (the red solid line) transforms from 'suppressed' state to 'conducted' state. This means that only one spin-polarized channel opens and the current is highly spin-polarized. Which spin channel (the up-spin channel or the down-spin channel) has contribution is depended on the leads contact locations. So we can achieve one types of spin-polarized current by adjusting the positions of the leads.

Table1. The Mulliken spin population at each carbon site of pristine ZGNR. The signs of spin populations indicate up-spin and down-spin respectively.

	Spin population							
Site	W=1	2	3	4	5	6	7	Total
1	-0.6944	+0.1582	-0.067	+0.158	-0.067	+0.1582	-0.6944	-1.0184
2	+0.729	-0.103	+0.0608	-0.0555	+0.0608	-0.103	+0.729	+1.3181

According to the convention labeling spin states, the up edge zigzag row is mainly the down-spin states. Why the down-spin channel is completely suppressed near the Fermi lever when the leads link to the 1-1□ site? By adopting the Mulliken population analysis (Table 1), we can clearly see that the spin populations are the largest at the edge carbon (the armchair sides) which due to the unsaturated electron-rich edge carbon. The total spin population of the up edge zigzag row (R1-zigzag row) is -1.0484, and in the second zigzag row (R2-zigzag row) is +1.3181, which is consistent with the spin population that we set. The signs ＋ and － indicate different spin populations. It is known that the spin population discussed above is the case for the valence band states. However, we usually study the electronic behavior of the conduction band which is an opposite case compared with the valence band states. This is why the up-spin channel is conducted while the down spin-channel is completely suppressed when the electrodes are contacted to the R1-zigzag row.

We now consider the transport properties after introducing single boron to the pristine ZGNR, one important feature appears in the transmission spectra. Whether the electrodes contact locations at 1-1 site or 2-2 site, the up-spin/down-spin channel is increase up to $1G_0$ at the Fermi level, while the down-spin/up-spin channel almost keeps unchanged. So the spin-polarization effect is enhanced near the Fermi level after inducing boron atom. This feature can be understood as follows: when the boron atom is doped at the R1-zigzag row where the up-spin states are localized, it injects a hole that will be filled with an up-spin electron mainly from the nearby carbon atoms; thus making the up-spin channel increased at the Fermi level, while keeping the down-spin channel unchanged. When the boron atom is doped at the R2-zigzag row where the down-spin states are localized, it also injects a hole that will be filled with a down-spin electron; thus making the down-spin channel increased at the Fermi level, while keeping the up-spin channel unchanged. So, we can realize fully spin-polarized current near the Fermi level through boron doping.

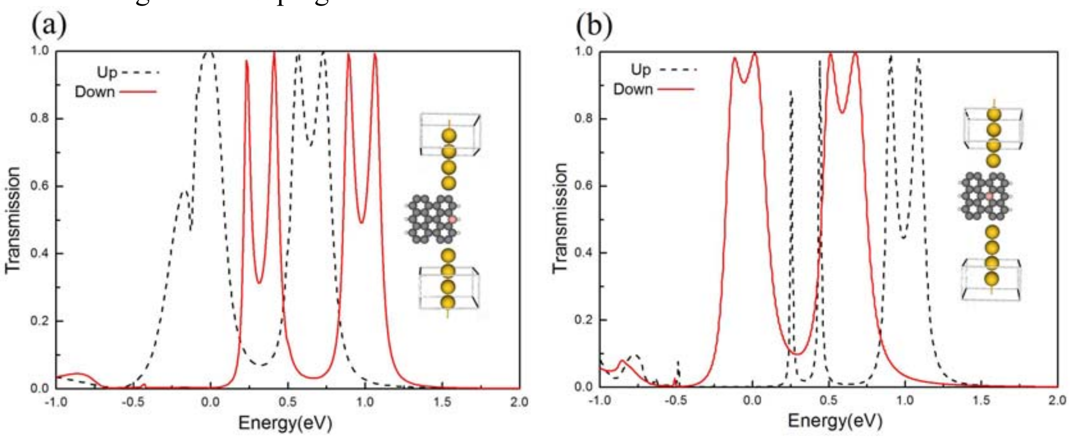

Figure 3. (Color online) Spin-dependent transmission spectrums of the boron doped pristine ZGNR. The insets show the contact geometries of electrodes (a) 1-1 site, (b) 2-2 site.

In order to obtain the physical picture for energy-dependent spin polarization of the transmission probabilities, we introduce spin polarization η and define it as:

$$\eta = \frac{T_{up} - T_{down}}{T_{up} + T_{down}}$$

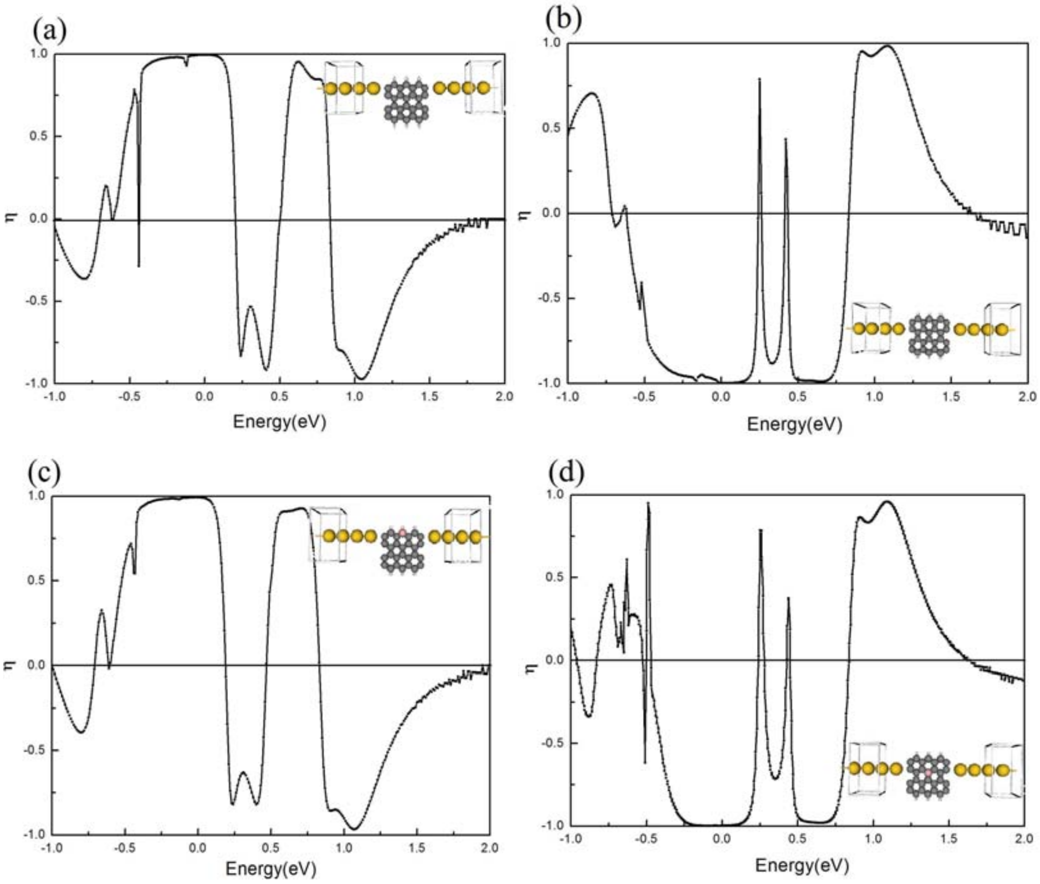

Figure 4. Spin polarization for pristine ZGNR in function of energies. The structures of Fig. 1 (b) are given as insets.

Figure 4 presents the spin polarization η as a function of energy. Compared Fig. 4 (a) to (b), the spin polarizations for both structures are very high at the Fermi level. However for the geometries of Fig. 1 (b), the η is a negative value which is due to the leads are linked to the edge where down-spin states are located. When the boron atom is doped at the ZGNR, the spin polarization is enhanced near the Fermi level, almost up to 100% [see Fig.4 (c) and (d)].

4. Conclusion

In this paper, we have calculated the device of the pristine ZGNR linked to linear Au atomic chains leads. The results show that when the electrodes contacts to one of the zigzag rows, we can obtain almost completely spin-polarized current. As the leads positions change from 1-1□ site to 2-2□ site, the up-spin transmission would transforms from 'conducted' state to 'suppressed' state, and the down-spin channel changes from 'suppressed' to 'conducted' state. So the type of spin-polarized current can be manipulated by changing the leads positions. For the boron doped ZGNR, this effect is enhanced, thus 100% spin-polarized current can be realized.

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