Controllable spin-dependent transport in the pristine graphene nanoribbons

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Abstract. Based on the non-equilibrium Green’s function in combination with the density-functional theory, we investigate the spin-dependent electronic transport of graphene nanoribbon partially linked to two single Au atomic chains leads with symmetry and asymmetry structures. For symmetry structures, the spin-dependent electronic transports are spin degeneracy, but for asymmetry structures, the spin degeneracy will be broken, leading to high spin polarization. So the spin-polarized transport can be controlled simply by adjusting connection structure between leads and graphene nanoribbon ends. Deeper analyses indict that the spin-dependent transport behaviours can be interpreted by the magnetic moments and the local density of state (LDOS).

1. Introduction
Graphene nanoribbon (GNR) have attracted great interests in quantum electronic devices because of their electronic structure [1,2], and transport properties[3,4], especially the zigzag GNR (ZGNR) with spin-polarized ground states have been most intensely studied [5-7]. Due to the pristine ZGNRs are completely spin degeneracy, we cannot get spin-polarized current. Therefore, in order to generating a spin-polarized current, some methods have been proposed to modulate spin transport properties in the ZGNR, for example, external electrical field [8], introducing vacancy defect or doping [9-12], making use of molecule adsorption[13,14] and graphene nano-junctions[15,16] etc. The results revealed that the structure of pristine ZGNRs linked partially to two semi-infinite leads is also a good method for tuning the spin-polarized transport properties of GNR [17].

In this letter, we consider the structure of pristine ZGNR partially linked with two leads of Au chains. It is revealed that the connection locations of the leads have enormous influence on the spin polarization transport properties. As the left and right leads are contacted symmetrically to the pristine ZGNR, the spin-polarized transport is completely spin degeneracy. As the left and right leads are linked asymmetrically to the pristine ZGNR, completely spin-polarized transport is received. The magnetic moments and the local density of states (LDOS) of the devices can the above phenomenon.

2. Computational method and model
We calculate the transport properties of two types of structures (Fig. 1, where the Gray balls represent Carbon, white balls represent Hydrogen, the yellow balls represent Au). Figure 1(a) and (b) are the pristine ZGNR symmetrically contacted on the Au atomic chains, Figure 1(c) and (d) are the pristine ZGNR asymmetrically contacted on the Au atomic chains, and each structure is two linking ways.

The total transmission probability $T(E)$ can be decomposed into the spin-dependent $T_{\sigma}(E)$,
For each spin state $\sigma$ the spin-dependent transmission spectra $T_\sigma(E)$ at energy $E$ is expressed as

$$T_\sigma(E) = T[R\Gamma L G^a TR G\Gamma]_\sigma,$$  

(2)
Fig. 2 describes the transmission spectrums $T(E, V_b)$ with $V_b=0$ for all the four systems given in Fig. 1. From the figure, we find that the contact positions obviously influence the transport properties. From the transmission spectrum of the symmetry structure [Fig. 2 (a), (b)], it can be seen that the transmission spectrums of both spins are completely degenerate, the two spin channel (spin-up and spin-down) are almost blocked at the Fermi level. Interestingly, for the asymmetry structure, the two spin transmission spectrums are completely separated at Fermi level [Fig. 2 (c), (d)]. Only one spin channel (up or down) is conduct, the other spin orientation transmission is suppressed, i.e. the up-spin channel exhibits an ‘ON’ state, and the down-spin channel exhibits an ‘OFF’ state for As1 [Fig. 2 (c)], it is just the opposite case compared to the structure of AS1, the up-spin channel is completely suppressed while the down-spin channel is conducted. Thus almost 100% spin polarization is realized by changing the contact locations.

![Graphical representation of transmission spectrums](image)

Fig. 3. (Color online) The circle on each carbon atom represents the magnetic moment, and the radius represents the size of the magnetic moment, where the black circle and the red circle represent the spin up and spin down respectively.

The different transport properties of the two types of structures can be understood by the magnetic moments of the pristine ZGNR shown in Fig. 3. We can clearly see that the populations are maximal at the edge carbon atoms due to the unsaturated electron of the edge carbon atoms. When the two leads are contacted symmetrically to the pristine ZGNR, the left and right edge carbon atoms connected with the leads have almost the same spin magnetic moment, but the spin direction is opposite. This is why the transmission spectrums of both spins are completely degenerate for the structures of S1 and S2. When the left and right leads are contacted asymmetrically to the pristine ZGNR, two carbon atoms connected to the leads have the same spin magnetic moment, and both the spin orientation is up-spin for As1, so the up-spin channel makes big contribution to the spin transport while the down-spin channel is completely blocked. For As2, it is just the opposite case compared to As1, the down-spin channel is conducted due to the carbon atoms connected to the leads have the same down-spin magnetic moment.

![Graphical representation of magnetic moments](image)

Fig. 4. (Color online) (a) and (b) Spin polarization for As1 and As2 systems in function of energies.
Figure 4 presents the spin polarization $\eta$ as a function of energy. Compared Fig. 4(a) to (b), the spin polarizations for both systems are very high at the Fermi level. However for the structures As1 and As2, the $\eta$ is the opposite sign, which is due to the leads are linked at the edge where up-spin states are located for As1 in Fig. 4(a), while in Fig. 4(b), the down-spin states are located at the edge.

**Fig.5.** (Color online) (a)-(d) The spin-dependent local density of state at the Fermi level with the symmetry and asymmetry structures.

To explain the above interesting transport phenomenon for the structures, we present the spin-dependent local density of state (LDOS) at the Fermi level with the symmetry and asymmetry structures, as shown in Fig. 5(a)-(d). The up-spin and down-spin LDOS are very small for symmetry structures, leading to the up-spin and down-spin transmissions are suppressed at the Fermi level (Fig. 5(a) and (b)). For As1 with the asymmetry structure, the up-spin transmissions are conducted while the down-spin transmissions are suppressed shown in figs. 5(c). However, for As2 with the asymmetry structure, it is just the opposite case compared to As1, the LDOS of up-spin is very small but the spin-down channel is very large. This indicates that the asymmetry structure can produce complete spin polarization compared with magnetic symmetry structure.

4. Conclusion

In conclusion, we study the spin-depended transport properties of pristine ZGNR linked to leads of Au chains with the symmetry and asymmetry structures. For symmetry structures, it is clearly seen that the transmission spectrums of both spins are completely degenerate with S1 and S2 structures. While for asymmetry structures, the spin separation effect can be achieved in As1 and As2 structures. But the electronic transmission of the up-spin channel are conduct and the down-spin channel are suppressed for As1 structure, for As2 structure, it is just the opposite case compared to the structure of As1, the up-spin channel is almost suppressed and the other is conducted. Thus, the spin-polarized transport can be controlled by adjusting the linking way between leads and pristine ZGNR.

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