Charge and spin transport in graphene-based heterostructure

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We investigate electron transport properties of a heterostructure based on zigzag graphene nanoribbons (ZGNR) by first-principles calculations. This heterostructure consists of hydrogen-terminated ZGNR (ZGNR-H) and oxygen-terminated ZGNR (ZGNR-O). We find that both charge and spin transport can be well controlled with the ZGNR-H/ZGNR-O heterostructure. A large charge transmission gap appears near the Fermi energy, and rectification behavior is observed. Moreover, the ZGNR-H/ZGNR-O heterostructure operates near the Fermi energy and rectification behavior is observed. Our results show that the ZGNR-H/ZGNR-O heterostructure hold promise for combining magnetoelectronics and conventional charge-based electronics. © 2011 American Institute of Physics. [doi:10.1063/1.3549154]

Graphene has attracted much attention in recent years due to its unique properties.¹ Zigzag graphene nanoribbons (ZGNRs) are particularly interesting.²–¹⁰ Some significant ZGNR-based models have been proposed, such as valley filter,²,³ half-metallic ZGNRs,⁴–⁷ and giant magnetoresistance (GMR) devices.⁸,⁹ Recent experiments demonstrate that graphene nanoribbons can be unzipped from carbon nanotubes.¹⁰ The final products prefer zigzag edges which are most likely to be terminated by oxygen. It is thus possible to fabricate hydrogen-terminated ZGNR/oxygen-terminated ZGNR (ZGNR-H/ZGNR-O) heterostructure using a mask to selectively reduce these oxygen-terminated ZGNRs. In this letter, we study electron transport properties of a ZGNR-H/ZGNR-O heterostructure. We find that both charge and spin current can be well controlled with the ZGNR-H/ZGNR-O heterostructure. A large transmission gap near the Fermi energy and rectification behavior is observed. Moreover, the ZGNR-H/ZGNR-O heterostructure operates as a perfect bipolar spin filter and exhibits GMR effect.

Our calculations are based on first-principle method with ATK package.¹¹ Geometry optimization is performed using VASP code until the force becomes less than 0.01 eV/Å. The vacuum layers between two sheets along the z and x directions (defined in Fig. 1) are 15 Å. The Perdew–Zunger exchange and correlation functional within the local density approximation is used. A cutoff energy of 150 Ry and a Monkhorst–Pack k-mesh of $1 \times 1 \times 100$ are chosen, and single-$\zeta$ polarized basis set is adopted for electron wave function. The NRGF-DFT self-consistency was controlled by a numerical tolerance of $10^{-5}$ eV.

Figure 1 shows the schematic configuration of a ZGNR-H/ZGNR-O heterostructure. Due to different electronegativity of edge atom, the Fermi level of ZGNR-H is different from that of ZGNR-O. The equilibrium state of the ZGNR-H/ZGNR-O heterostructure is then realized by electron transfer, which mainly takes place at the three ZGNR-H units ($H_1$, $H_2$, and $H_3$) and the two ZGNR-O units ($O_1$ and $O_2$) around the ZGNR-H/ZGNR-O interface as shown in the top panel of Fig. 2(a). The negative (positive) value of transferred electron represents the decreased (increased) electron population on each unit. The electron transfer is also reflected in the density of states (DOS) analysis. As shown in the middle panel of Fig. 2(a), the closer ZGNR-H unit to the interface, the smaller the sharp peak of DOS at the Fermi energy, indicating that the transferred electron originated from the delocalized $\pi$ orbital of ZGNR-H. The electron transfer into an unoccupied orbital of ZGNR-O unit near the interface can be seen from the bottom panel of Fig. 2(a), in which the nearest two ZGNR-O units ($O_1$ and $O_2$) to the interface show enhanced (reduced) DOS below (beyond) the Fermi energy compared with the third unit away from the interface. When equilibrium is reached, the band structure around the interface will be bent, resulting in a barrier as shown in Fig. 2(b). The top panel of Fig. 2(b) shows the eigenstate under a low bias (0.02 V). We can see that the presence of a barrier at the interface have little effect on electron transport. The injected electrons accumulate near the interface and tunnel through this barrier. Therefore, the underlying mechanism of determining the transmission is the electron tunneling between ZGNR-H and ZGNR-O electrode as shown in the bottom panel of Fig. 2(b).

In Fig. 3(a), we show the conductance of a ZGNR-H/ZGNR-O heterostructure. As a reference, we show in dashed and dotted lines the conductances of ZGNR-H and ZGNR-O, respectively. Both the ZGNR-H and the ZGNR-O show good conductivity within the energy range $-2 < E - E_F < 2$ eV. However, in the case of the ZGNR-H/ZGNR-O heterostructure...

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FIG. 1. (Color online) The schematic illustration of ZGNR-H/ZGNR-O heterostructure. $H_i$ or $O_i$ ($i = 1\text{--}N$) means the $i$th unit away from the interface.
ture, the electron transmission in the vicinity of the Fermi energy is highly asymmetric. When \( E < E_F \), the conductance is near 1 \( G_0 \). However, a large transmission gap is open when \( E > E_F \). The bottom left (right) panel in Fig. 3(a) shows the open (blocked) eigenchannel at \( E - E_F = -0.2 \) eV and \( E - E_F = 0.2 \) eV, respectively. In order to clarify the mechanism of current tunneling, the band structure of ZGNR-H and ZGNR-O electrode is shown in Fig. 3(b). The band structure of edge oxidized ZGNRs in the right panel of Fig. 3(b) shows three open channels around the Fermi level because there are two bands crossing the Fermi level, one of them being the \( \pi^* \) band and the other being the doubly degenerate O-\( \pi \) lone-pair band. Only the \( \pi^* \) band contributes to the electron transport because only \( \pi \) and \( \pi^* \) band appear near the Fermi level in the ZGNR-H electrode. It has been reported that orbital symmetry of ZGNRs strongly affect the transport properties under bias.\(^8,14\) Our eigenstate analysis [see the inset in the right panel of Fig. 3(b)] shows that the \( \pi^* \) subband of ZGNR-O is \( C_2 \) symmetry which is different from the \( \pi^* \) subband of ZGNR-H. Therefore, a large transmission gap appears when the energy is larger than Fermi energy. The current-voltage characteristic of this ZGNR-H/ZGNR-O heterostructure displays rectification effect as shown in the Fig. 3(c).

Next, we study spin transport properties of ZGNR-H/ZGNR-O heterostructure. All three spin configuration (nonmagnetic, antiferromagnetic, and ferromagnetic) of ZGNR-O yield the same bandstructure.\(^8,15\) Thus, spin transport through ZGNR-H/ZGNR-O heterostructure can be represented by the \([1,0]\) or \([-1,0]\) configuration, where \( 1 \) (\(-1\)) represents the magnetization of ZGNR-H electrode and \( 0 \) represents the nonmagnetic state of ZGNR-O electrode. As shown in Fig. 4(a), within the energy range \(-0.2 < E - E_F < 0.25 \) eV, the spin down channel is open while the spin up channel is completely suppressed. Consequently, as shown in Fig. 4(b), the spin down current shows metallic behavior and the spin up current is completely blocked, demonstrating a perfect spin filter effect. Obviously, the result of spin-splitting in the \([-1,0]\) configuration is opposite to that of the \([1,0]\) configuration and leads to the spin up polarization around the Fermi energy. Interestingly, as shown in Fig. 4(c), combining the properties of spin and charge transport gives rise to GMR effect. In the \([0,0]\) configuration, the charge current increases slowly with increasing positive bias voltage and eventually saturates when the bias voltage is larger than 0.05 V, indicating a very high differential resistance \((dV/dI)\). In the \([1,0]\) configuration, the total spin current increases much more quickly and remains linear when the bias voltage increases, indicating a relatively low differential resistance \((dV/dI)\). The inset of Fig. 4(c) shows the bias-dependent MR can be as high as 800%.

In summary, our first-principle studies on the transport properties of the ZGNR-H/ZGNR-O heterostructure show that the ZGNR-H/ZGNR-O heterostructure integrates several useful functions on controlling both charge and spin current. Due to its simple structure and the advances in ZGNR fabrication, ZGNR-H/ZGNR-O heterostructure hold promises for future carbon-based electronics.

\(^5\)E.-J. Kan, Z. Li, J. Yang, and J. G. Hou, Appl. Phys. Lett. 91, 243116
FIG. 3. (Color online) (a) Transmission spectrum (solid line) of the ZGNR-H/ZGNR-O heterostructure. The transmission spectrum of ZGNR-H (dashed line) and ZGNR-O (dotted line) are used as a reference. The bottom panel shows the open and blocked eigenchannels at $E-E_F=-0.2$ eV and $E-E_F=0.2$ eV, respectively. (b) Band structure for the ZGNR-H lead (left panel), transmission curve (middle panel), and band structure for the ZGNR-O lead (right panel) for charge transport at zero bias. The inset in the right panel shows the isosurface plot of the wave functions for ZGNR-O. (c) $I$-$V$ curves for the ZGNR-H/ZGNR-O heterostructure.

FIG. 4. (Color online) (a) Spin-dependent electron transmission of the ZGNR-H/ZGNR-O heterostructure at zero bias for the magnetic [1,0] configuration. (b) $I$-$V$ curves for the ZGNR-H/ZGNR-O heterostructure with magnetic configurations of [1,0]. The inset shows the bias-dependent spin polarization, calculated by $100 \times \frac{(I_{up}-I_{down})}{(I_{up}+I_{down})}$. (c) $I$-$V$ curves for both charge and spin transport of the ZGNR-H/ZGNR-O heterostructure under a small bias. The inset shows that the calculated MR can be as high as 800% calculated by $100 \times \frac{(dV/dI)_{10}-(dV/dI)_{10}}{(dV/dI)_{10}}$. 

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