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Resonance induced spin-selective transport behavior in carbon nanoribbon/nanotube/nanoribbon heterojunctions

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ABSTRACT

Carbon nanotubes (CNTs) and graphene nanoribbons (GNRs) are attractive in spintronics. Here, we propose GNR/CNT/GNR heterojunctions constructed by attaching zigzag-GNRs at the side-wall of CNT for spintronic devices. The thermal stability and electronic transport properties were explored using *ab initio* molecular dynamics simulations and nonequilibrium Green's function methods, respectively. Results demonstrate that the sp^3-hybridized contacts formed at the interface assure a good thermal stability of the system and make the CNT to be regarded as resonator. Only the electron of one spin-orientation and resonant energy is allowed to transport, resulting in the remarkable spin-selective transport behavior at the ferromagnetic state.

1. Introduction

Graphene and carbon nanotubes (CNTs) are nano carbon materials with novel mechanical, thermal, electronic, and optical properties [1,2]. Especially the extraordinarily high electronic mobility and long spin-lifetime provide them with great potential applications in molectronics and spintronics [3–6]. Chemically bonding CNT and graphene together is a promise route to use those novel properties for practical device applications [7–14]. For example, by growing CNTs on graphene sheets [15], the obtained CNT–graphene materials show outstanding properties superior to either CNTs or graphene alone [16–18]. Another type of graphene–CNT materials can be obtained by growing graphene nanosheets/leaves on the side-wall of CNTs randomly, which shows their remarkable optoelectronic and gas-sensing properties [19,20]. By partially unzipping CNTs [21–23], the resultant CNT/graphene-nanoribbon (CNT/GNR) heterojunctions can possess many interesting properties, such as electronic rectifier, half-metal, quantum interference and magnetoresistance [7,21–26].

GNR/CNT/GNR heterojunctions can be obtained by cutting the graphene–CNT obtained by growing graphene on the side-wall of CNTs [19,20]. Differing from the CNT/GNR heterojunction obtained by partially unzipping CNTs, sp^3-hybridized contacts exist at the interface between GNR and CNT. But how the sp^3-hybridized contacts affect the transport properties of GNR/CNT/GNR heterojunctions remains unclear. Actually, sp^3-hybridized contacts are always present in covalently functionalized graphene, fullerene, and CNTs materials [27–29], which show promising applications in supercapacitor, photovoltaic device, and electrochemical catalysis [12,13,19,20,27,30]. Understanding the effect of sp^3-hybridized contacts on the transport properties of GNR/CNT/GNR also relates to the practical applications of these materials.

In this work, the good thermal stability of GNR/CNT/GNR heterojunctions was proved using *ab initio* molecular dynamics stimulations (ab-MD) at room temperature, and an efficient spin-selective transport behavior was revealed from first principles calculations, suggesting potential applications of the heterojunctions in spin injection and spin filter devices. It is revealed that the sp^3 contacts play a crucial rule in determining the thermal stability and transport properties of GNR/CNT/GNR heterojunctions.

2. Models and methods

To examine the width dependence, the GNR/CNT/GNR with three different widths ($N = 6, 8, 10$) was considered, where the N is identified as the width of the GNR and is the number of zigzag lines contained in the GNR. To eliminate dangling bonds of the system, all the edge C atoms were terminated by H atoms. The central scattering region (CSR) was consisted of the whole CNT section and five unit cells of GNR at each side. The CSR was also used as the extending molecule in ab-MD simulations. A large enough vacuum layer was used to eliminate the interaction between the system and its mirror images, as shown in Fig. 1(a) and (b).

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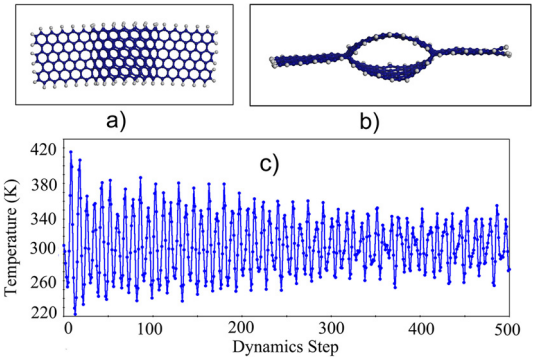

Fig. 1. (a) and (b) are top view and side view of the GNR/CNT/GNR with width $N = 6$, which are grabbed from the ab-MD stimulations at 500 fs. (c) shows the fluctuation of temperature as the function of dynamics steps.

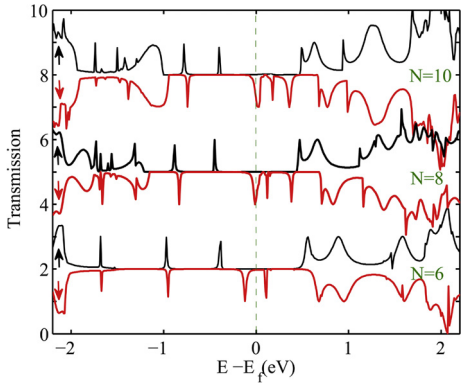

Fig. 2. (Color online.) Zero-bias spin-polarized transmission spectra of the three GNR/CNT/GNR heterojunctions at FM state. For clarifying, the curve of the system with $N = 6$, 8, and 10 are shifted up for 2, 5, and 8 units, respectively.

The ab-MD simulations, structural optimizations, electronic structure, and electronic transport properties were calculated by performing SIESTA 3.2 package [31]. Nose–Parrinello–Rahman thermostat at room temperature was used in simulations. Spin-polarized density functional theory (DFT) was utilized for structural optimizations and electronic structure calculations. A double-ζ plus polarization (DZP) basis set was employed in DFT calculations, with an energy shift parameter of 0.01 Ry that determines the cutoff radii of atomic orbitals. A revised Perdew–Burke–Ernzerhof (rPBE) [32] functional of generalized gradient approximation (GGA) was used for the exchange correlation potential [33]. The residual force was controlled with a tolerance of 0.002 eV/Å on each atom. Electronic transport was calculated using nonequilibrium Green's functions (NEGFs) in combination with spin-polarized DFT, in which the exchange correlation was also taken into account by rPBE-GGA.

3. Results and discussion

To meet the requirements of electronic device minimization, the size of GNR/CNT/GNR heterojunctions should be small to molecular and nano scales. We examined the thermal stability of the system at room-temperature with the width at molecular scale by performing ab-MD simulations. The simulation process stops at 500 steps with a step length of 1 fs. The final structure of the system with width $N = 6$ was grabbed using VMD [34], and the top-view and side-view were plotted in Fig. 1(a) and (b), respectively. Fig. 1(c) is the fluctuation of the simulation temperature as the function of dynamics steps. One can notice that with the simulation going on, the fluctuation of temperature decreases gradually and closes to 300 K, but the junction keeps its structure very well. Indicated that the system has a good thermal stability even it works at room temperature.

After examined the thermal stability, we optimized the structure and calculated the total energy of the system at non-polarized (NP) state and spin-polarized state with anti-ferromagnetic (AFM) or ferromagnetic (FM) configurations, respectively. We find that just like pure zigzag GNRs, AFM is the ground state of the system. For the system of $N = 6$, the calculated energy difference between NP and AFM states ($\Delta E_1 = E_{NP} - E_{AFM}$) is *29.91 meV* per edge-C atom, and the ΔE between AFM and FM states ($\Delta E_2 = E_{AFM} - E_{FM}$) is *18.1 meV* per edge-C atom. The ΔE_1 and ΔE_2 for $N = 8$ are *32.47 meV* and *10.4 meV*, and for $N = 10$ are *36.61 meV* and *4.27 meV*, respectively. Obviously, the ΔE_1 increases with the width increasing, suggesting the spin-polarized ground state even of the system with a wide width. While the ΔE_2 decreases with the width increasing, suggesting that FM and AFM are energetically almost degenerated in wide junction. Considering FM state can be easily achieved by the applying of electric field [35], we explore transport properties of the system at FM state only.

The zero-bias spin-polarized transmission spectra of the system were plotted in Fig. 2. One can see very sharp transmission peaks around the Fermi level of each system, indicating a remarkable resonant transport feature. This is hardly surprising by noting that two sp^3-hybridized linear contacts present at the interface between CNT and GNR. Due to the insulating characteristics of sp^3-hybridized C atoms, the two sp^3 contacts can act as electronic isolators and the CNT between the two isolators can be regarded as a resonator [36]. It only allows the electrons with resonant energies to transport through the system [37], resulting in the sharp transmission peaks.

Moreover, each system has obviously asymmetrical transmissions between spin-up and spin-down electrons due to the spin polarization. One can see that up-spin electron has a wide zero-transmission gap of 0.7 eV at the Fermi level, and the gap does not change its value with the width of the junction increasing. While down-spin electron has a few resonant transmission peaks very close to or right at the Fermi level. This means that the system possesses an insulating behavior for one spin orientation but a metallic behavior for the other. Moreover, the resonant peaks move close the Fermi level with the width of the junction increasing, this is due to the fact that the variance of width changes the inherent frequency of the resonator. Hence, the spin-selective behavior observed here should also present the junctions even with a wide width. Previous studies indicated that a wide spin-splitting occurs only near the Fermi level of the zigzag-GNRs at FM state [38,35]. Our calculations suggest that the energy of up-spin electron near the Fermi level locates at the forbidden region of the CNT resonator, thus its transmission is almost zero. While, the down-spin electrons have different energies from the up-spin electrons due to the spin-polarization, the down-spin electron with appropriate energy is allowed to resonantly transport through the junction. Such a remarkable spin-selective transport behavior is very useful for realizing all-carbon spin injection and spin filter devices in spintronics [35,39].

To unveil the underlying origin of such a useful spin-selective transport, we chose the CSR with width $N = 6$ as the supercell and calculated its spin-polarized charge density. The top-view and side-view of the iso-surface of the obtained density near the Fermi level were plotted in Fig. 3(a) and (b), respectively. Normally, the pin-polarization mainly occurs at the edge C atoms of the system. Taking the top edge as the example, one can see that just like pure zigzag GNRs, the "A" and "B" sublattices near the edge contribute to the transmission eigenstates of down-spin and up-spin electrons, respectively. While each "A" sublattice has a much heavy density than the "B" sublattice due to spin polarization.

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