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Designing cross-linked carbon nanotubes as perfect spin filter and spin valve

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ABSTRACT

By applying nonequilibrium Green's functions in combination with density-function theory, the spin-dependent transport properties of cross-linked carbon nanotube spintronic devices are investigated. Our calculations show that the perfect spin filtering effect with the almost 100% spin polarization, and the magnetoresistance effect with a magnetoresistance ratio larger than 10^4% can be observed in the device. The occurrence of the perfect spin-filtering and magnetoresistance effects in the cross-linked carbon nanotube spintronic device provides the possibility for further improving the integration level of carbon nanotube networks. Moreover, the mechanisms for these interesting phenomena are suggested.

1. Introduction

Spintronic devices with low energy consumption and high speed have attracted the attention of many researchers. At present, people's interests mainly focus on the design and development of spintronic devices. Meanwhile, many spin transport phenomena, such as spin filtering effect [1–3], magnetoresistance (MR) effect [4–6], spin crossover [7], Kondo effect [8], etc., have also been found in the spintronic devices. These interesting physical phenomena can endow the spintronic devices with the functions of logical operations and information storage. Therefore, designing the spintronic devices with interesting spin transport phenomena is our current goal.

So far, many kinds of molecular materials have been chosen to construct the spintronic devices, such as carbon nanotubes (CNTs) [9–12], C_{60} [13,14], graphene nanoribbons [15–18], zigzag α-graphyne nanoribbons [19], boron nitride nanoribbons [20], n-acenes family [21], etc. Especially, CNTs have greatly stimulated the interest of researchers due to their long phase-coherence and spin scattering lengths. Many efforts have been devoted to designing CNTs-based spintronic systems. For instance, Urdampilleta et al. [9] designed a CNT-based supramolecular spin valve, and found MR ratio up to 300%. Mehrez et al. [10] reported a CNT magnetic tunnel junction which is composed of single-wall CNT and ferromagnetic electrodes. They observed a MR phenomenon with a MR ratio ranging up to 20%. Using *ab initio* modeling, Huang et al. [11] observed spin-filtering effect in a CNT/FeN_4 complexes/CNT molecular junction. All these systems listed above display spin-filtering or MR effects, which shows profound potential for designing as the spin-filter or spin valve. At present, however, how to obtain the high spin-polarization and MR ratios for CNTs-based spintronic devices by an effective design method is still an interesting topic due to the fact that the ratio is a key index for the practical application of the devices. Motivated by the research content in Refs. [22,23], we design a high-performance spintronic device by using the cross-linked CNTs.

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Our results show that perfect spin-filtering and MR effects can be observed in the device. Therefore, our research work provides a possible avenue to achieve the perfect molecular spin filter and spin valve.

2. Model and formalism

The cross-linked CNTs systems we investigate are shown in Fig. 1. In the present study, we take the armchair (5,5) CNT as an example to investigate the transport properties of cross-linked CNTs. According to the previous reports [22,23], we consider two cross-linked ways in this study: (I) the nitrogen-doped CNTs are connected by the pyridine-like defect/Vanadium (V)/pyridine-like defect structure [see the Fig. 1(a)]; (II) the CNTs are connected by the η^6-coordinated V atom [see the Fig. 1(b)]. To facilitate discussion, the devices in the Fig. 1(a) and (b) are called as M1 and M2, respectively. For M1 (M2), the two V atoms are separated by a large distance. Thus, their spin directions can be modified independently under the external magnetic field [24,25]. If the spin directions of two V atoms in the M1 is set in parallel (antiparallel), the corresponding magnetic configuration is denoted as $M1_{\uparrow\uparrow}$ ($M1_{\uparrow\downarrow}$). Similar to M1, M2 can be also set as two different magnetic configurations, namely, $M2_{\uparrow\uparrow}$ and $M2_{\uparrow\downarrow}$. In the present work, we study the spin-dependent transport properties of $M1_{\uparrow\uparrow}$, $M1_{\uparrow\downarrow}$, $M2_{\uparrow\uparrow}$ and $M2_{\uparrow\downarrow}$, and thus assess the effect of connection ways between CNTs on transport properties in the cross-linked CNTs systems. The structures have been optimized and the spin transport properties are calculated by the first-principles method based on the fully self-consistent *ab initio* density-functional theory [26,27]. The spin transport properties of the cross-linked carbon nanotube are interpreted by using Landauer formula [28]

$$I_\sigma(V_b) = \frac{e}{h}\int_{\mu_L}^{\mu_R} T_\sigma(E, V_b)dE, \tag{1}$$

where the σ is the spin index (spin up = ↑; spin down = ↓); μ_L and μ_R indicate the chemical potentials of left and right electrodes, respectively, and the difference between them is eV_b. $T_\sigma(E, V_b)$ is the spin-resolved transmission probability defined as

$$T_\sigma(E, V_b) = Tr[\Gamma_L G^R \Gamma_R G^A]_\sigma, \tag{2}$$

where $G^{R(A)}$ is the retarded (advanced) Green functions of the central region.

3. Numerical results and discussion

Fig. 2 presents the spin-dependent currents as a function of applied bias for all magnetic configurations. We can find from Fig. 2(a) that with the increase of the bias, the spin-up and spin-down currents of $M1_{\uparrow\uparrow}$ rise quickly. Similar case can also be seen in $M1_{\uparrow\downarrow}$. This means that both spin-up and spin-down states for $M1_{\uparrow\uparrow}$ ($M1_{\uparrow\downarrow}$) present the metallic characteristic under finite bias. Thus, the spin

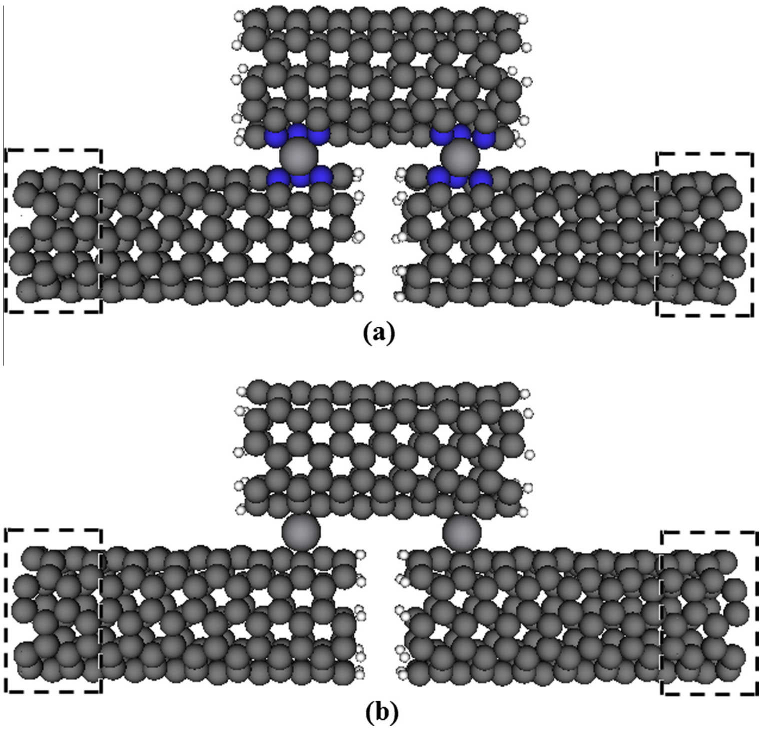

Fig. 1. (a) [(b)] A schematic of M1 [M2]. Blue and white spheres indicate nitrogen and hydrogen atoms, respectively. Gray spheres sandwiched between CNTs are vanadium atoms. The CNT in the dashed box is the electrode part of the system, which is described by a supercell with two repeated carbon unit cells along transport direction. If the spin directions of two vanadium atoms in M1 [M2] is set in parallel (antiparallel), the system is named as $M1_{\uparrow\uparrow}$ ($M1_{\uparrow\downarrow}$) [$M2_{\uparrow\uparrow}$ ($M2_{\uparrow\downarrow}$)]. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)