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Contact transparency inducing negative differential resistance in nanotube–molecule–nanotube junction predicted by first-principles study

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ABSTRACT

We construct a molecular junction where propyl contacts two armchair carbon nanotubes through five-member ring and perform the first-principles calculations of its transport properties. The negative differential resistance effect with peak-to-valley ratio of 700% is present. Our investigations indicate that contact transparency can induce negative differential resistance in nanotube–molecule–nanotube junction, which may promise the potential application in nano-electronics devices in the future.

1. Introduction

Negative differential resistor (NDR, i.e. Esaki diode or tunneling diode [1] in the traditional electronics devices) has wide applications such as amplifiers, logic cells, memories, etc. Since Chen et al. [2] and Xue et al. [3] have discovered the NDR effect in thiol molecules contacting gold lead via scanning tunneling microscopy, molecular and nano-scale NDRs attracted much investigational interesting due to that molecular and nano-scale devices are considered as the potential substitutes of traditional Si-based semiconductor transistors in the future. Especially, carbon nanotubes (CNTs) based NDRs [4–36] are the center of attention because CNTs are excellent materials to construct molecular and nano-scale devices. Ke et al.'s calculations [37] indicate that near-perfect contact transparency is present in the CNT–molecule–CNT junctions where molecules contact CNTs via a five-member ring, which motivates us to propose that contact transparency can induce NDR effect under low bias. Here, according to the first-principles studies of the CNT–propyl–CNT transport system where propyl contacts (5, 5) CNT via a five-member ring, our proposal is confirmed. In our previous studies, we proposed that the charge distribution and the localization of energy states can induce NDR and rectification behavior [38–40]. Here, we find that the contact transparency in the molecular junctions may also induce NDR behavior under low bias.

2. Computational details

Our calculations are based on a self-consistent first-principles method of non-equilibrium Green's function combining density functional theory. The code we use is the Atomistix Toolkit [41–44]. The k-points sampling is 1, 1, and 50 in the x, y, and z direction. The cutoff energy and basis set is 150 Ry and SingleZeta, respectively. The exchange-correlation interaction is treated within generalized gradient approximation using the Perdew–Burke–Ernzerhof functional [45]. The convergence criterion for the total energy is 10^{-5} via the mixture of the Hamiltonian. The currents are calculated as

$$I = \frac{2e}{h}\int_{-\infty}^{+\infty} T(V_b, E)\big[f_L(E-\mu_L) - f_R(E-\mu_r)\big]\,dE \tag{1}$$

where $f_{L,R} = 1/(1+e^{(E-\mu_{L,R})/k_BT})$ is the Fermi–Dirac distribution; $\mu_{L,\,R}$ are the chemical potentials of the left lead (L) and the right lead (R). h is Planck constant, V_b is bias and $T(V_b, E)$ is transmission coefficients. Fig. 1 shows the schematics of transport system constructed by two (5, 5) CNTs sandwiching propyl. The propyl contacts to (5, 5) CNT via a five-member ring (or in other words,

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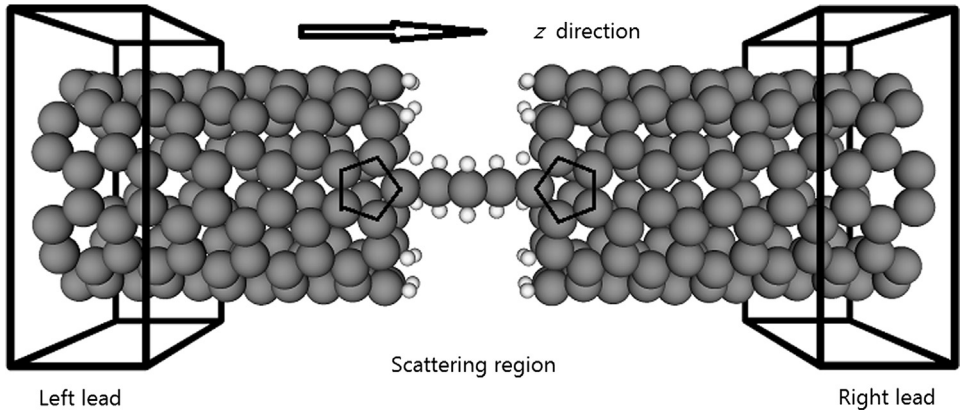

Fig. 1. Schematics of transport system of two (5, 5) carbon nanotubes sandwiching propyl. Black pentagon in the scattering region indicates the position of carbon five-member ring. The whole transport system is divided to left lead, scattering region and right lead. Color code: C atom (black) and H atom (grey).

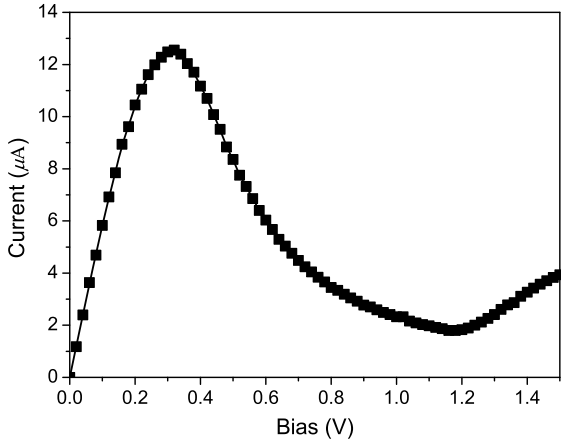

Fig. 2. The curves of the bias-dependent current for transport system.

via an apex carbon atom). The scattering region is relaxed until the force tolerance of 0.02 eV/Å is achieved.

3. Results and discussions

Fig. 2 shows the current–voltage (I–V) curve of the transport system. From Fig. 2, one can see the current rapidly increases until the bias is 0.32 V. After 0.32 V, the current decreases until the bias is 1.16 V. The NDR behavior is present and the peak-to-valley ratio [PVR, here, it is the ratio between current peak and current valley and defined as $I_{\text{peak}}(V_b = 0.32\ \text{V})/I_{\text{valley}}(V_b = 1.16\ \text{V})$] is as large as 700%.

Studying the bias-dependent $T(V_b, E)$ spectra, density of states (DOS) spectra and local DOS can help us to penetrate the mechanisms which result in the I–V characteristics. Fig. 3(a) and 3(b) respectively shows the DOS and $T(V_b, E)$ spectrum at several biases. From Fig. 3(a), for zero bias, one can see that there is a broad DOS peak around Fermi level. Following the DOS spectrum, there is a high and broad $T(V_b, E)$ peak around Fermi level at zero bias [shown in Fig. 3(b)]. Such $T(V_b, E)$ peak demonstrates that contact transparency of carbon five-member ring not only present in π conjugated molecules [37] but also in σ bonded molecules. Fig. 3(c) shows the local DOS at -0.06 eV where the $T(V_b, E)$ peak locates for zero bias. From Fig. 3(c), one can clearly see that the local DOS is mainly composed by the p_x states on the apex carbon atoms. In the following, we call these p_x states on the two sides of σ barrier are incident and transmitted p_x state from left to right.

When the bias is applied to leads [$+V_b/2$ ($-V_b/2$) is applied to left (right) lead], the electrochemical potential in the left (right) lead is shifted down (up) by $V_b/2$. Because separated by σ barrier, the incident (transmitted) p_x state around Fermi level shift down (up) rough following the left (right) lead. That is to say, the energy difference between incident and transmitted p_x state increases as bias increases. From Fig. 3(a), as the bias increases, one can see that the DOS peak around Fermi level gradually divide to two low DOS peaks. The DOS peak is splitting and hasn't yet formed two independent DOS peaks before the bias of 0.56 V. After 0.56 V, The DOS peak absolutely divide to two independent DOS peaks. Such two independent DOS peaks are contributed by the incident and transmitted p_x states. Actually, the I–V characteristics are the results of the mutual competition of two mechanisms when the bias is applied to leads. The first mechanism is that the transport window (i.e., the part of the transmission function in the bias window integrated to obtain the current. It is the energy region from $-eV_b/2$ to $+eV_b/2$) enlarges with the bias increases, which will increase the current; The second one is that $T(V_b, E)$ around Fermi level shrink as the bias increases, which will decrease the current. Let us qualitatively explain the second mechanism. When the bias increases, the incident (transmitted) p_x state shift down (up) as mentioned above. The coherent tunneling transport is present when the carrier waves propagate between incident and transmitted p_x state. When the energy difference between incident and transmitted p_x states is small, the $T(V_b, E)$ contributed by coherent tunneling around Fermi level are large enough. Otherwise, if such energy difference is large, the $T(V_b, E)$ contributed by coherent tunneling will decrease. To more clearly explain the second mechanism, the incident and transmitted p_x state can be known as two series "transmission channels". The mismatching of two series "transmission channels" at energy presentation destroy the $T(V_b, E)$ and eventually decreases the current [As shown in Fig. 3(a), the DOS peak dividing to two DOS peaks also means the mismatching of two series "transmission channels" at energy presentation as bias increases]. We see Fig. 3(b) and find that the $T(V_b, E)$ peak around Fermi level indeed becomes low and broad as the bias increase because the energy difference between incident and transmitted p_x state increases mentioned above. For the discussions above, the reason which causes the NDR behavior of the transport system is clear. When the bias is between 0.00 and 0.32 V, the first mechanism beat the second one and results in that the current increases. When the bias is between 0.32 and 1.16 V, the second mechanism beat the first one and results in that the current decreases.

Based on the results and discussions, in the field of molecular and nano-scale electronics, we propose a method to produce NDR behavior under very small bias. In the molecular and nano-scale