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Effect of length and size of heterojunction on the transport properties of carbon-nanotube devices

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By applying nonequilibrium Green’s functions in combination with the density-functional theory, we investigate the electronic transport properties of molecular junctions constructed by the mirror symmetrical straight carbon-nanotube heterojunctions. The results show that the length and size of heterojunction play an important role in the electronic transport properties of these systems. The negative differential resistance behavior can be observed in such devices with certain length and size of heterojunction. A mechanism is suggested for the negative differential resistance behavior.


In the past decade, molecular devices constructed by carbon nanotubes have attracted much attention. The electronic transport properties of carbon-nanotube devices have been studied experimentally,1,2 and theoretically.3–7 It is known that an ideal single-walled carbon nanotube (SWNT) can be either a metal or a semiconductor, depending on its helicity and diameter. A joining of two or more distinct nanotubes with different helicities and diameters, by introducing pentagon-heptagon defect pairs into the perfect hexagonal network,8 will produce a carbon-nanotube heterojunction. The electronic characteristics of semiconductor/metal and metal/metal heterojunctions have been investigated experimentally9–11 and theoretically.12,13 The carbon-nanotube Y-junctions14 and T-junctions,15 and superlattice nanotube structures16 have also been reported. However, most of these studies mainly focused on the electronic properties of carbon-nanotube heterojunctions (CNTHs), while the transport behavior of metal electrode/carbon-nanotube heterojunctions/metal electrode devices (MCNHM) were paid less attention.

In this present work, by applying nonequilibrium Green’s functions and first-principles calculations, we investigate the electronic transport properties of MCNHM modulated with different CNTH configurations, as shown in Fig. 1. The structures have been optimized and the quantum transport calculations have been carried out by an ab initio code package, TRANSIESTA-C.17 TRANSIESTA-C is based on the real-space, nonequilibrium Green’s function formalism and the density-functional theory. The main feature of the computational package is to model a nanostructure coupled to external electrodes with different electrochemical potentials and to realize the transport simulation of the whole two-probe system. Our results show that electronic transport properties of the devices may be modulated by the size and length of the heterojunction. Moreover, a negative differential resistance (NDR) is observed and tuned by the length and size of the heterojunction. The NDR is a very useful property in electronic devices such as molecule switch. The NDR behavior has been found in mesoscopic systems such as double barrier quantum wells18 and superlattices.19,20 The resonant18 and off-resonant19 electronic tunneling mechanism have been proposed to explain the NDR behavior. NDR has also been found in a number of molecular devices. Several groups observed the NDR in a phenylene ethynylene trimer substituted by nitro and amino groups on the central ring.21–24 A possible mechanism such as a two-step reduction process,21 the change of the molecular conformation due to the change of the electronic charge state of the molecule under increasing bias,22–24 a bias-induced alignment of the molecular orbitals,24 and side groups effects24 for the NDR in such a system have also been proposed by these groups. The NDR was also observed in a single benzene ring with a NO2 ligand.25,26 D. Ventra et al. attributed the NDR to the rotation of the ligand activated by temperature,25 while Luo and Fu suggested that a one-electron reduction is the mechanism behind the NDR.26 Phonon-mediated NDR in suspended carbon-nanotube molecular wires has also been reported.27,28 In analogy to a quantum double-dot structure, Liu et al. showed that molecular-level crossing in an organometallic molecular double-dot system can lead to NDR.29 Recently, we investigate the electronic transport properties of MCNHM modulated with different CNTH configurations, as shown in Fig. 1. The structures have been optimized and the quantum transport calculations have been carried out by an ab initio code package, TRANSIESTA-C.17 TRANSIESTA-C is based on the real-space, nonequilibrium Green’s function formalism and the density-functional theory. 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The main feature of the computational package is to model a nanostructure coupled to external electrodes with different electrochemical potentials and to realize the transport simulation of the whole two-probe system. Our results show that electronic transport properties of the devices may be modulated by the size and length of the heterojunction. Moreover, a negative differential resistance (NDR) is observed and tuned by the length and size of the heterojunction. The NDR is a very useful property in electronic devices such as molecule switch. The
Bandyopadhyay and Wakayama found that NDR could be
generalized and tuned in the junctions of a Rose Bengal
molecule.30 In spite of a number of theoretical and experi-
mental studies about NDR in various kinds of molecular
devices, the origin for NDR is still under intense debate. Our
results show that the conduction channel being suppressed at
a certain bias is responsible for the NDR behavior in the
MCNHM systems considered here.

In Fig. 2, we show the transmission coefficient $T(E, V_b)$
at zero bias ($V_j=0$) for the two-probe systems shown in Fig.
1. From Figs. 2(a1)–2(a3), as expected, it is found that no
transmission gap (namely, zero transport flat) exists in the (6,
0) tube system, while a narrow and a wider transmission gap
exist in the transmission spectra of (7, 0) and (8, 0) tube
systems, respectively. This means that the (6, 0) tube system
is of a metallic behavior, while (7, 0) and (8, 0) tube systems
display a semiconducting behavior. When introducing a (7,
0) or (8, 0) tube into a (6, 0) tube, a metal/semiconductor/
semiconductor-nanotube heterojunction is formed. For such a
system, the transmission behavior is different from that of a
single (6, 0), (7, 0), or (8, 0) tube system. From Figs. 2(c1)–
2(c3), it can be found that transmission gap appears, and it
becomes wider with an increase of the number $N$ of cells of
the (8, 0) tube. It is known that an interface can form in the
matching region between (6, 0) and (7, 0) or (6, 0) and (8,
0) tubes. The electron transport through heterojunction is
dependent on the resonant coupling between different tubes.
For a single (6, 0) tube system, we find by calculation that its
transport channels [lowest unoccupied molecular orbital
(LUMO), highest occupied molecular orbital (HOMO), and
HOMO-1 to LUMO-5] lie within the energy gap of a single
(8, 0) tube. For (6, 0)/N(8, 0)/(6, 0) systems, when the system
contains only one cell of the (8, 0) tube, it is found by
calculation that only LUMO channels will be suppressed, so
a narrow transmission gap appears. When more cells of the
(8, 0) tube is contained in CNTH, more channels will be
closed, and the transmission gap becomes wider. From Figs.
2(b1)–2(b3), we find that for (6, 0)/N(7, 0)/(6, 0) systems,
the transmission coefficient is decreased with the number $N$
of cells of the (7, 0) tube, and a small transmission gap
appears when $N$ is 5. This results from the fact that the energy
gap of the (7, 0) tube is narrow and the geometric dis-
tortion is weak in the matching region between (6, 0) and
(7, 0) tubes.

Figure 3 describes the currents as a function of the applied
bias for MCNHM systems. From the figure, we can see clearly
that when the bias is larger than a certain threshold bias, the current can flow apparently in (6, 0)/N(7, 0)/(6, 0) systems,
and the value of the threshold bias becomes bigger when changing $N$ from 1 to 5, which indicates that these systems
are of semiconducting characteristics and they can be
modulated by the length of the junctions. However, for
(6, 0)/N(8, 0)/(6, 0) systems, there is a small zero-current flat
(about ±0.25 V) only when $N=5$. From the figure, we
find an interesting feature: The current decreases obviously
when the bias is between $|V| = 1.1$ V and $|V| = 1.3$ V for both
(6, 0)/3(7, 0)/(6, 0) and (6, 0)/1(8, 0)/(6, 0) systems, which
means NDR appears in the bias range in the these systems.
However, for other systems, we do not find the NDR behavior.
To understand the NDR behavior in our systems, we
calculated the transmission coefficient $T(E, V_b)$ of the
(6, 0)/1(8, 0)/(6, 0) system under biases $V_b=1.1$, 1.2, and
1.3 V, as shown in the inset in Fig. 3. It is clearly seen that
for $V_b=1.1$ V and $V_b=1.3$ V, there are three peaks in the
region of energy $E$ between 1.0 and 1.3 eV. However, only
two peaks appear in the transmission spectra in the region of
energy $E$ between 1.0 and 1.3 eV for $V_b=1.2$, which means
that the conduction channel at $E=1.04$ eV is suppressed.

To understand the origin of the peaks being suppressed
in transmission curves, in Fig. 4, we give the molecularly
projected self-consistent Hamiltonian (MPSH) at the eigen-
value $E=1.04$ eV of the (6, 0)/1(8, 0)/(6, 0) system for the
biases $V_b=1.1$, $V_b=1.2$, and $V_b=1.3$ eV, respectively.
Considering the fact that the Fermi level (energy zero) is varied with the bias, the levels of the molecular orbitals are also varied with the bias. By our calculation, at the energy $E=1.04$ eV, the
molecular orbitals correspond to LUMO+19, LUMO+19, and
LUMO+20 for the biases $V_b=1.1$, $V_b=1.2$, and $V_b=1.3$ V,
respectively. From Fig. 4(a), it can be found that when the bias is 1.1 V, the MPSH of LUMO+19 is delocalized, which shows that the conduction channel can make a larger contribution to
the current. As a result, a transport peak appears at the $E = 1.04$ eV for the bias of 1.1 V, as shown in the inset in Fig. 3. From Fig. 4(b), we can find that when the bias is 1.2 V, the MPSH of the channel LUMO+19 localizes on the left part of the structure, which means that the channel is suppressed. Consequently, the current at the bias of 1.2 V is smaller than that at the bias of 1.1 V. As the bias is further increased, the electronic current remains low due to LUMO+19 being suppressed. When the bias is increased to 1.3 V, channel LUMO+20 is opened, so a peak appears at the $E = 1.04$ eV again. This leads to the current being rapidly increased. So, whether the channel is opened or suppressed is responsible for the decrease of the current of the $(6,0)/(18,0)/(6,0)$ system at the bias being about 1.1 V in Fig. 3. In fact, this is the reason for NDR. A similar explanation is for the NDR behavior in the $(6,0)/3(7,0)/(6,0)$ system at the bias of 1.2 V. It should be noted that as long as not too many molecular orbitals contribute to the electron transport, the role of suppressed channel is obvious to the electron current, and so the NDR can be observed clearly. This is similar to the negative differential capacitance in the quantum dot. From our calculations, it is known that the NDR behavior can be observed only in the $(6,0)/(18,0)/(6,0)$ and $(6,0)/3(7,0)/(6,0)$ systems, while in $(6,0)/N(8,0)/(6,0)$ ($N=2$, 3, and 5) or $(6,0)/N(7,0)/(6,0)$ ($N=1$, 2, and 5) systems, the NDR does not occur for the explored bias range. These results show that the NDR behavior originates from the conduction channel being suppressed at a certain bias. Whether the channel is opened or suppressed depends on the length and size of the semiconductor tube in the molecular junction.

In summary, using first-principles quantum transport calculations, we have investigated the transmission properties of electrons in molecular junctions constructed by the mirror symmetrical straight carbon-nanotube heterojunctions with different sizes and lengths. The calculated results show that the size and length of the heterojunction play a significant role on the current-voltage characteristics. The NDR behavior can be observed in such devices and depends on the size and length of the heterojunction. It is suggested that the conduction channel being suppressed at a certain bias voltage is the origin of the NDR behavior.

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