Size effect of quantum conductance in single-walled carbon nanotube quantum dots

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Abstract. The quantum conductance of two kinds of carbon nanotube quantum dots (CNQD) composed of (5,5) and (10,0) tubes, namely (10,0)/(5,5)/(10,0) and (5,5)/(10,0)/(5,5) with different quantum sizes, are calculated. It is shown that for (10,0)/(5,5)/(10,0) CNQD, one on-resonant peak at the Fermi energy exists only for special QD sizes, and the width of the conductance gap increases from 1.0 eV to 3.2 eV with the increase of size. The positions of peaks around the Fermi energy are obtained by the electronic structure of individual finite (5,5) tubes. We also find that the (5,5)/(10,0)/(5,5) CNQDs behave as a quantum dot, and its localized QD states are different from that of the former CNQD because of the existence of the interface states between (5,5)/(10,0) junctions. For (5,5)/(10,0)/(5,5) CNQD, there is no conductance gap with QD’s size smaller than 7 layers, and the conductance peak around the interface quasilocalized state –0.26 eV disappears with QD sizes larger than 23 layers. In addition, for the (5,5)/(10,0)/(5,5) CNQD, the connection method can change the degree of electronic localization of intermediate (10,0) tube.

PACS. 61.48.+c Fullerenes and fullerene-related materials – 71.20.Tx Fullerenes and related materials; intercalation compounds – 72.80.Rj Fullerenes and related materials – 68.55.Ln Defects and impurities: doping, implantation, distribution, concentration, etc.

1 Introduction

The continual miniaturization of electronic devices has always been a major driving force in the microelectronic industry. The ultimate goal is to synthesize devices as small as possible, i.e. as small as a molecule or a cluster of atoms. Molecularly perfect materials such as single-wall carbon nanotubes (SWCNs) can provide new opportunities for designing nanometer-sized electronic devices.

SWCN can be either metallic or semiconducting depending on both the diameter and chirality, which can be uniquely determined by the chiral vector (n,m), where n and m are integers \cite{1}. If two nanotubes (one semiconducting and the other metallic) are connected, a heterojunction is formed which can act as a rectifying diode. Such two-terminal heterojunctions or rectifying diodes were first postulated theoretically \cite{2}, and recently observed in experiments \cite{3,4}. Transport measurements performed in SWCNs, which were deposited on metallic contacts \cite{5,6}, have given evidences of resonant tunnelling through quantized energy levels. Such reports stimulated several theoretical models of CNQDs. Recently, carbon nanotube Y-junctions were produced by Li et al. \cite{7}, and theoretically studied by \cite{8}. These tubular heterostructures called intramolecular heterojunctions (IMJs) offer new perspectives for nanoelectronic technology. Chico et al. \cite{9} first proposed that a quantum dot can be obtained by combining two carbon-nanotube metal-semiconductor junctions, which behaves as an ideal zero-dimensional device. Both the discrete nature and the spatial localization of the (5,5) tube-derived states unambiguously demonstrate quantum confinement. Therefore, the (6,4)/(5,5)/(6,4) system behaves as a quantum dot, and is thus called a carbon nanotube quantum dot (CNQD). The singular electronic properties of CNQDs may be important in future nanoelectronics, since a CNQD with metallic contacts could behave as a one-electron transistor, and Coulomb blockade effects due to occupation of these strongly localized discrete levels are expected. So it could be envisioned to integrate an electronic circuit of nanotube based architecture, where multi-terminal junctions or nodes have multifunctional logic characteristics. However, the detailed

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calculation of electron transport phenomenon through IMJs which include the influences of structure and size are required.

In this work, we have performed calculations of the electronic structure and quantum conductance of the (10,0)/m(5,5)/(10,0) CNQD, which is different from the (6,4)/(5,5)/(6,4) QDs studied by Chico et al. [9]. The size dependence of the QD states is investigated, as required for the design of a quantum device. Furthermore, we studied another type of CNQD, namely M/S/M (5,5)/m(10,0)/(5,5), which has three different topological configurations. The section between two semi-infinite SWCNs can be considered as one quantum dot. We also studied their general quantum characteristics, together with the dependence of the number and localization of bound states on the size of QDs. We adopted a tight-binding Hamiltonian and followed the single-particle Green’s function formalism to obtain LDOS within real-space renormalization techniques [10,11]. Given that electron transport on the molecular scale has become a topic of intense applications, we also calculated the conductance of CNQDs adopting the Landauer-Kubo formalism [12]. This work is organized as follows: in Section 2, we present the theoretical method. In Section 3, we proceed with the numerical calculations, and give discussions. Finally, the summary is given in Section 4.

2 Theoretical method

We perform the calculation of the local density of states (LDOS) and quantum conductance to characterize the electronic properties within a tight binding description of the carbon bonds. We use the following Hamiltonian

\[ H = \sum_{\langle i,j \rangle, s} V_{pp \pi} \left( C_{i,s}^\dagger C_{j,s} + C_{i,s} C_{j,s}^\dagger \right), \]

where \( \sum_{\langle i,j \rangle} \) is restricted to nearest-neighbor atoms, and \( V_{pp \pi} = -2.75 \text{ eV} \) is the two-center hopping integral. On-site energies are set to zero, therefore the Fermi energy \( E_F \) is zero. All the hopping parameters are equal, independent of the bond length, curvature, or any rearrangement due to the presence of defects. Therefore, the changes are solely induced by the alterations in the topology of the hexagonal rolled lattice.

The metallic contacts are realized by two different carbon nanotube (CNs) in order to investigate their roles in the conductance. Electronic correlations are neglected in this simple calculation, although they are relevant for a proper description of confined systems such as the proposed quantum dots. Since we consider a real-space Hamiltonian, the details of the atomic arrangement of the junction may be completely incorporated through an adequate microscopic description. Surface Green’s functions for the semi-infinite CNs are calculated through the solution of matrix-like Dyson equations obtained by successive decimations of unit cells. The average LDOS at ring \( j \) and energy \( E \) is given by \( \rho_j(E) = -1/(\pi n_j) \text{ImTr} G_{j,j}(E) \), where \( \text{Tr} \) stands for the trace over the \( n_j \) carbon atoms of ring \( j \), and \( G_{j,j}(E) \) refers to the Green’s function at ring \( j \). Let us consider a heterojunction \( C \) connected to two semi-infinite SWCNTs. The conductance is most conveniently solved using the Green’s function matching (GFM) method. A fundamental result in the theory of electronic transport is that the conductance through a region of interacting electrons is related to the scattering properties of the region itself via the Landauer formula: \( T = (2e^2/h) T \), where \( T \) is the conductance, and \( T \) the transmission function is expressed as such

\[ G_C = (E - H_C - \Sigma_L - \Sigma_R)^{-1} \]

where \( \Sigma_L,R \) are the self-energy terms due to the semi-infinite SWCNTs, and \( H_C \) is the Hamiltonian of the heterojunction. The self-energy terms also define the coupling \( \Gamma \) through the following relation:

\[ \Gamma_{L,R} = i \left[ \Sigma_{L,R}^a - \Sigma_{L,R}^p \right]. \]

In turn, the self-energy terms are calculated with a previously published surface Green’s function matching technique [13].

3 Results and discussion

First, we calculate the electronic properties and quantum conductance of a single (5,5)/(10,0) interface. To confirm the resonant behavior of the system, we plot both quantum conductance and the local density of electronic states (LDOS) together in Figure 1. The energy range of interest is from 0.45 eV to 0.45 eV around the semiconductor gap of the infinite (10,0) tube. The quantum conductance gap of the interface (5,5)/(10,0) is from -1.6 eV to 1.6 eV as determined by the (5,5) tube, which is larger than the band gap of the semiconducting segment (about 1 eV). The larger conductance gap is due to the mismatch in the conducting states of the (5,5) and (10,0) segments. The presence of 5–7 defect leads to a different LDOS for the conduction and valence bands. Even though one sharp peak in the LDOS for the (5,5)/(10,0) interface, is observed in the gap region, there is no peak in the gap region of quantum conductance. This shows that the interface quasiloclized states are off-resonance states. The basic characteristics of the LDOS and quantum conductance are in agreement with the results of Rochefort et al. [14], where they studied the quantum size effect of finite (5,5)/(10,0) junction between two gold leads using the