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Simulation of STM technique for electron transport through boron-nitride nanotubes

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ABSTRACT

We report first-principles calculations on the electrical transport properties of boron-nitrid nanotubes (BNNTs). We consider a single walled (5, 0) boron-nitrid nanotube sandwiched between an Au(1 0 0) substrate and a monatomic Au scanning tunneling microscope (STM) tip. Lateral motion of the tip over the nanotube wall cause it to change from one conformation class to the others and to switch between a strongly and a weakly conducting state. Thus, surprisingly, despite their apparent simplicity these Au/BNNT/Au nanowires are shown to be a convenient switch. Experiments with a conventional STM are proposed to test these predictions. The projection of the density of states (PDOS) and the transmission coefficients $T(E)$ of the two-probe systems at zero bias are analyzed, and it suggests that the variation of the coupling between the wire and the electrodes leads to switching behaviour.

1. Introduction

The next generation of electronic devices will undoubtedly be constructed of molecules, or have features of molecular size. The results of recent experimental [1–3] and theoretical studies [4–11] predict a brilliant future for molecular electronics. Among various efforts and activities, several schemes have been proposed to design and construct molecular switches [3,8–11]. The basic idea is to find molecules that have two or more distinct states with vastly different conductance. Switching between *on* and *off* states can be performed by applying an external bias or by using a scanning tunneling microscope tip to manipulate the system [3,8–11].

The transport properties of carbon nanotubes have attracted much attention because of possible applications for nanodevices [12,13]. Many experiments have demonstrated that single-wall nanotubes exhibit ballistic and coherent electron conduction, with the phase relaxation length larger than the typical tube length of a few micrometers [14,15].

Several theoretical [13,16–18] and experimental [19–22] studies has elucidated various aspects of electron transport through Metal/Nanotube/Metal junctions. However the possibility that wires of this type may be capable of switching is far from obvious a priori and has not been investigated until now.

Thus as well as identifying the simplest two-terminal molecular switch to date and shedding new light on the mechanisms of molecular switching, the present work reveals an unexpected new dimension of the physics of Au/BNNT/Au junctions.

The molecular switch that we describe should be amenable to experimental study with presently available techniques. Thus our findings also raise the prospect of bridging the gap that has persisted in this field between theory and experiment since molecular switching was first observed.

2. Computational details

The calculations have been performed using a recently developed first-principles package SMEAGOL [23,24], which is based on the combination of DFT (as implemented in the well-tested SIESTA method [25]) with the NEGF technique [26,27]. SMEAGOL is capable of fully self consistently modeling the electrical properties of nano-scale devices that consist of an atomic scale system coupling

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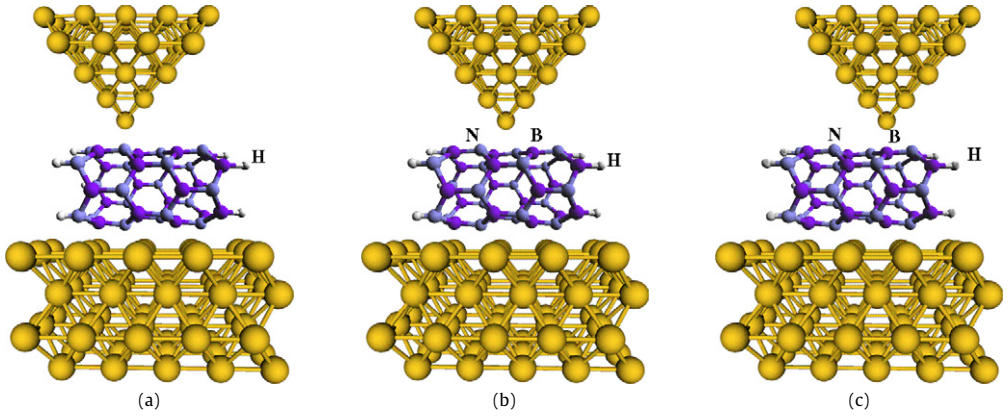

Fig. 1. A schematic of a single walled (5, 0) boron nanotube (SWBNNT) sandwiched between two Au(1 0 0) electrodes according to the scanning tunneling microscope (STM) technique. (a) The N-link conformation, (b) *hollow* conformation and (c) B-link conformation.

with two semi-infinite electrodes. Such nano-scale devices are referred to as two-probe systems and they are divided into three parts for theoretical calculations: left and right electrodes, and a central scattering region. The scattering region actually includes a portion of the semi-infinite electrodes. The simulation procedure of such two-probe systems can be described briefly as follows.

Firstly the electronic structure of two electrodes is calculated only once by SMEAGOL to get a self-consistent potential. This potential will be shifted rigidly relative to each other by the external potential bias and provides natural real space boundary conditions for the Kohn–Sham (K–S) effective potential of the central scattering region. Then from the Green's function of the central scattering region, it can obtain the density matrix and thereby the electron density. Once the electron density is known, the DFT Hamiltonian matrix, which is used to evaluate the Green's function, can be computed using the above boundary conditions by means of standard methods.

$$\hat{G} = \lim_{\delta\to 0}\left[(E+i\delta)\hat{S} - \hat{H}_{S[\rho]} - \hat{\Sigma}_L - \hat{\Sigma}_R\right]^{-1}, \tag{1}$$

where $\hat{H}_{S[\rho]}$ is DFT Hamiltonian and $\hat{\Sigma}_L$ and $\hat{\Sigma}_R$ are the self-energies respectively for the left and right lead. This procedure is iterated until self-consistency is achieved. Moreover, the current through the atomic scale system can be calculated from the corresponding Green's function and self-energies using Landauer–Buttiker formula [28]

$$I(V) = \frac{2e}{h}\int_{-\infty}^{+\infty} dE\left[f_l(E-\mu_l) - f_r(E-\mu_r)\right]T(E,V), \tag{2}$$

where μ_l and μ_r are the electrochemical potentials of the left and right electrodes respectively, i.e.,

$$\mu_L - \mu_R = eV_b \tag{3}$$

and f_r, f_l are the corresponding electron distribution of the two electrodes. $T(E,V)$ is the transmission coefficient at energy E and bias voltage V, which is given by

$$T(E,V) = \mathrm{Tr}\left[\mathrm{Im}\,\Sigma_l(E)G^R(E)\,\mathrm{Im}\,\Sigma_r(E)G^A(E)\right], \tag{4}$$

where $G^R(E)$ and $G^A(E)$ are the retarded and advanced Green's function of the central region. Based on the eigenchannel decomposition of the conductance, this total transmission $T(E)$ can be decomposed into nonmixing eigenchannels $T_n(E)$ [29] as

$$T(E) = \sum_n T_n(E). \tag{5}$$

In our DFT calculation, the local-density approximation (LDA) to the exchange-correlation potential [30] is used. Only valence electrons are considered in the calculation, and the wave functions are expanded by localized numerical (pseudo) atom orbitals (PAOs) [31]. The atomic cores are described by norm-conserving pseudo potentials [32].

The initial structure model of the (5, 0) BNNT was a cluster-type consisting of 40 boron and nitrogen atoms. The dangling bonds at both ends were tied off with hydrogen atoms, yielding a B_{20} N_{20} H_{10} tube. In this two-probe system, BNNT was sandwiched horizontally between two atomic scale Au(1 0 0) electrodes which extend to reservoirs at $\pm\infty$ where the current is collected. Three Au atomic layers have been chosen for the electrode cell in the z-direction. In the central scattering region the BNNT couples with three atomic layers to the bottom side and with the STM tip, which was represented by a tetrahedron of Au atoms, to the top side. These atomic layers in the central scattering region are large enough [33] so that the perturbation effect from the scattering region is screened and they are denoted as surface-atomic layers. The structural model for our theoretical analysis is illustrated in Fig. 1.

In order to investigate the switching behaviour of the BNNT, we consider three conformations for the BNNT attached to the Au electrodes. In the first conformation, the STM tip was placed above the N atom of the BNNT (N-link conformation) (Fig. 1(a)). In the second conformation, the Au tip atom was placed over the hollow site of the hexagonal ring of the BNNT (*hollow* conformation), as depicted in Fig. 1(b). Finally, in the third conformation, the STM tip was placed above the B atom of the BNNT (B-link conformation), as shown Fig. 1(c).

3. Results and discussion

In recent years, much progress has been made developing theories of electron transport through molecules [34–44]. An important conclusion has been that the current at low bias is carried by molecular orbitals. The overlap between the orbitals and the states of the contacts is sensitive to the orientation of the molecule relative to the contacts, which implies a strong orientation-dependence of the molecular wire's conductance [11,40]. Such overlap effects have been found in semi-empirical [36,41] and density functional [38] transport calculations.

Thus, it is reasonable to expect them to result in a significant change in conductance when an Au-BNNT-Au wire switches between various conformations, and our calculations show this to be the case. Since DFT calculations have been successful in explaining the experimental current-voltage characteristics of SWBNNTs bonded to gold electrodes [13,41,42,44] we adopted this approach here. In Fig. 2, we show the calculated current of the BNNT in its ground state conformation for three positions of the STM tip along