صفحه ۱ تا ۹

Study of I–V in CNT zigzag BN nanotube

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Abstract

We numerically investigate the conductance properties and I-V characteristics of (n, 0) zigzag single-walled nanotubes. In the BN/CNT/BN structure using a tight-binding model and some well-known approaches and methods based on Green's function theory and Landauer formalism, where nanocontacts are of as (n,0) zigzag single-walled carbon nanotubes. We compare them in three cases when n= (8, 0), n= (14, 0), and n= (16, 0). We calculate the value of Dos in a tight-binding Hamiltonian way in its case when for the three cases when the shape of the tube is zigzag and knowing the voltage and current for each case. We perform the calculations theoretically using MATLAB program. We investigate the conductivity and I-V characteristics of zigzag (n, 0) single-walled BN nanotubes in a BN/CNT/BN structure using Landauer formalism and Green's function theory. Electronic band structures and density of states of (n, 0) for (8, 14, 16) carbon nanotubes in the presence of different amount of B and N impurities were calculated. It was found that these impurities have significant effect on the conductivity of carbon nanotubes. The electronic properties of small gap semiconducting (n, 0) tube can extensively change in the presence of impurity. Our results indicate that B-doped and N-doped (n, 0) carbon nanotubes can be p- and n-type semiconductors, respectively.

Introduction

Research on the study and manipulation of matter at the nanoscale is booming, and it has significant technological ramifications. To depict the molecular system and the reservoirs, numerous theoretical studies have been created and models put forth. The molecular wires were typically two semi-infinite surfaces or two semi-infinite 'rods' [1, 2]. or one-dimensional sandwich transition metal-anthracene molecular wires [3], Simple molecular wires have been used in several recent efforts to join two semi-infinite carbon nanotubes (CNTs) [5,6].

The excellent electrostatics made possible by a nanotube electrode shape is responsible for the much better switching properties of short organic field effect transistors with metallic CNT electrodes compared to those with metal electrodes [7]. CNTs and hetero-materials, such as boron (B) and

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nitrogen (N), have drawn a lot of interest in both basic science and the development of nanotechnology devices [8]. Although CNTs can be metallic or semiconducting depending on their chirality, it has been calculate that heterojunctions of B-C-N nanotubes at n= (8, 0), n= (14, 0), and n= (16, 0) are generally independent of the radius, helicity, multiplicity, or degree of perfection of the constituent nanotubes [9]. By using electrical arc discharge [10], pyrolysis, and laser ablation techniques, BN nanotubes have been successfully synthesized [11].Therefore, BNNTs have poor electro-conductivity with insulator characteristics [12]. We have studied the effect of impurity on electronic properties of single-walled carbon nanotubes Following these interests and working towards the modelling of a molecular wire. We performed a model in this paper where two semi-infinite zigzag single-walled CNTs are used as nanocontacts to connect a zigzag single-walled BN nanotube**.**

Methodology

We calculate H0 for the unit cell, which consists of four lines, and each line consists of six cells n = (6, 0), where H0 was represented by a Hamiltonian matrix. We calculate DOS from estimating of the current values of zigzag shaped nanotube. We evaluate the H0 value by a tight-binding Hamiltonian method in three index of n (n, 0), when n= 8, n= 14 and n=16 by knowing the voltage and current for each case. We performed the calculations theoretically using MATLAB software. The most commonly used computational schemes for calculating the (coherent) conductance g are the Landauer theory [13], Green's function formalism tight binding method and Hamiltonian matrix [14,15]. The conductance g at zero temperature is simply proportional to the transmission coefficient, T (E), for injected electrons at the Fermi energy.

We could calculate the above submatrices of Green's function by solving the equation. This results in the following expression for Green's function in the device region:

We model the transport problem by dividing the system in three parts (Fig. 1): Two semi-infinite leads (L) and (R) with bulk electronic structure are connected to a finite region called device (D). The D region contains the scattering region (S) where the potential landscape for the electrons deviates from that in the leads, and a finite part of each lead (1) and (1). The leads' parts inside D are chosen sufficiently big such that the leads only couple to that part of the device. The Hamiltonian matrix is divided into submatrices as follows

$$H = \begin{pmatrix} H_L & H_{LD} & 0 \\ H_{DL} & H_D & H_{DL} \\ 0 & H_{RD} & H_R \end{pmatrix} \qquad (1)$$

Where it has been assumed that the electrodes do not directly interact which each other (H_{LR}=0=H_{RL}) as the D region is sufficiently big, or rather the electrode parts inside D as mentioned above. Green's function matrix is given by

$$G = \begin{pmatrix} G_L & G_{LD} & G_{LR} \\ G_{DL} & G_D & G_{DR} \\ G_{RL} & G_{RD} & G_R \end{pmatrix} \quad (2)$$

We could calculate the above submatrices of Green's function by solving the equation

$$(E - H)G(E) = 1 \quad (3)$$

This results in the following expression for Green's function in the device region

$$G_D\,(E) = (E - H_D - \sum_L(E) \sum L - \sum_R(E)^{-1} \quad (4)$$

Also the electronic density of states (DOS) and the current of the device are given as [16]:

$$DOS\,(E) = \frac{-1}{\pi}\, Im\,\{Tr\,[G\_D\,(E)] \quad (5)$$

$$I(v) = (2e/\,h\,) \int_{\mu_L}^{\mu_R} d\varepsilon T(\varepsilon)[f_L(\varepsilon) - f_R(\varepsilon)] \quad (6)$$

Results and discussion

CNT might be either metallic or semiconductor and the diameter and helicity of a nanotube are determined by the chiral vector (n, m), where n and m are integers. Theory predicted that when (n, 0) is divisible by 3, the CNT will be semiconductor. CNTs have small band gaps (E_g) in the range 0.2–2.0 eV, while BNNTs have much wider band gaps of about 5.5 eV, which are almost independent on their structures.

1 DOS (n,0) index

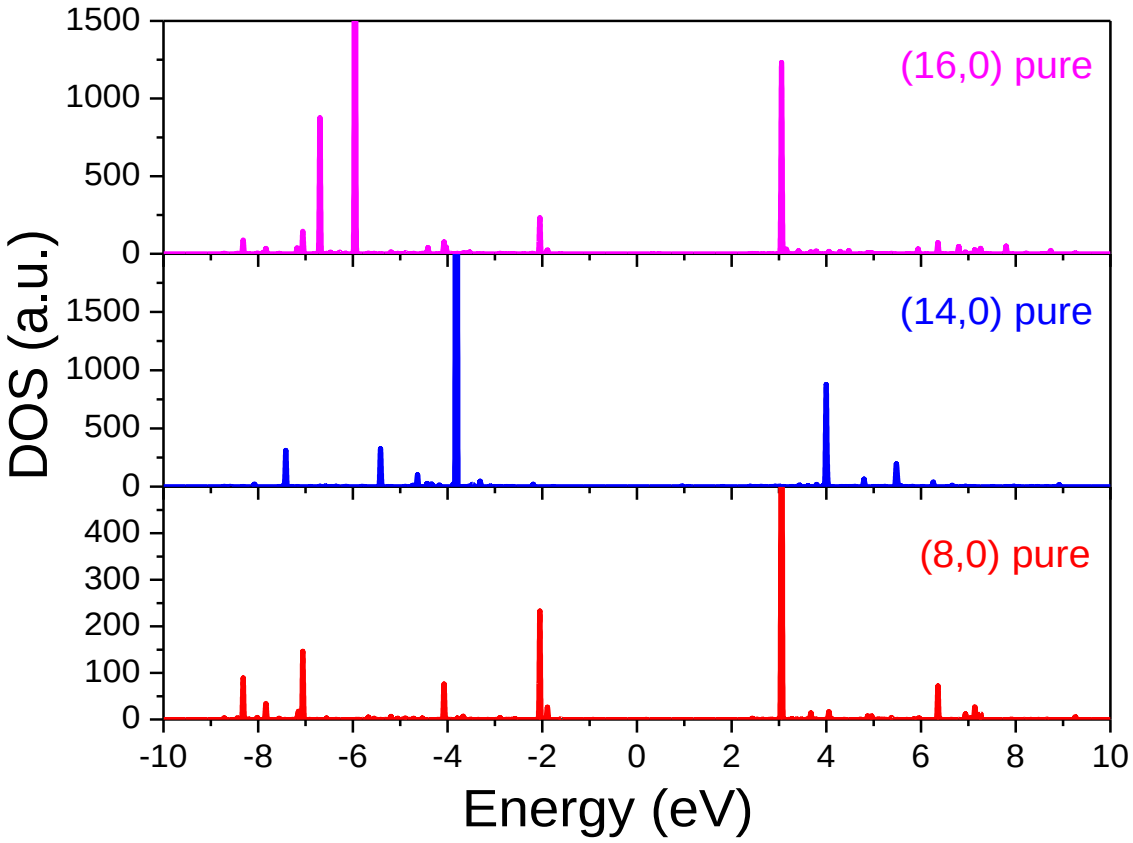

Figure of at (8, 0)

(14,0)and (16,0) in pure states.

Figure 1 shows the electronic density of the three states (DOS) in the BN / CNT/ BN system. We have studied the effect of impurity on electronic properties of single-walled carbon nanotubes using Tight-Binding Hamiltonian. Electronic band structures and density of state, carbon nanotubes in the presence of different amount of B and N impurities were calculated then, the current values for the three cases were calculated as shown in Figure 2-3-4.

The following (Figure 2) shows the density OF state (DOS) after adding B or N impurities to the system in the case when n = (8,0) between 5 and 6 unit cells .

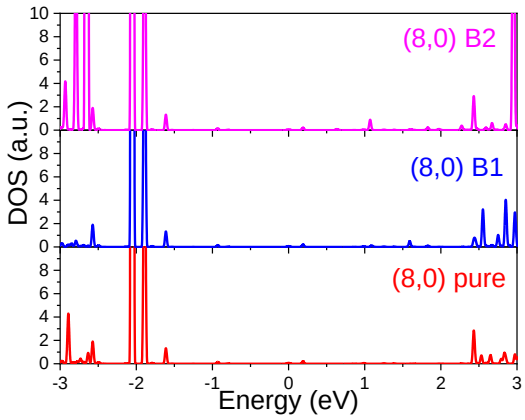

Figure 2 DOS of (n, 0) for pure and N and B impurity states in 5 and 6 unit cell at (8, 0)

We carried out the same operation, but with n (14,0), In the following figure (Figure 3), it shows the density after adding B or N impurities to the system in the case when it is between 5 and 6 unit cells.

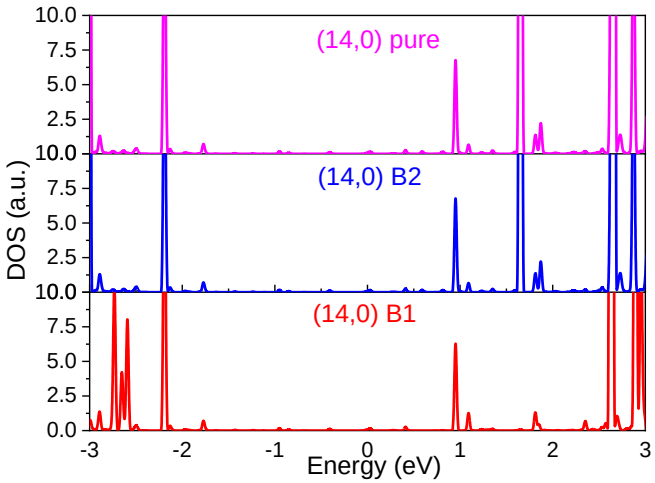

Figure 3 DOS of (n, 0) for pure and N and B impurity states in 5 and 6 unit cell at (14, 0)

The following(Figure 4) shows the electronic density of state (DOS) of n(16,0) in the CNT /BN /CNT system creating electronic states within the band gap, and this is shown by our diagrams in the previous two figures, which shows that pure nanotubes of type BN are semiconductors.

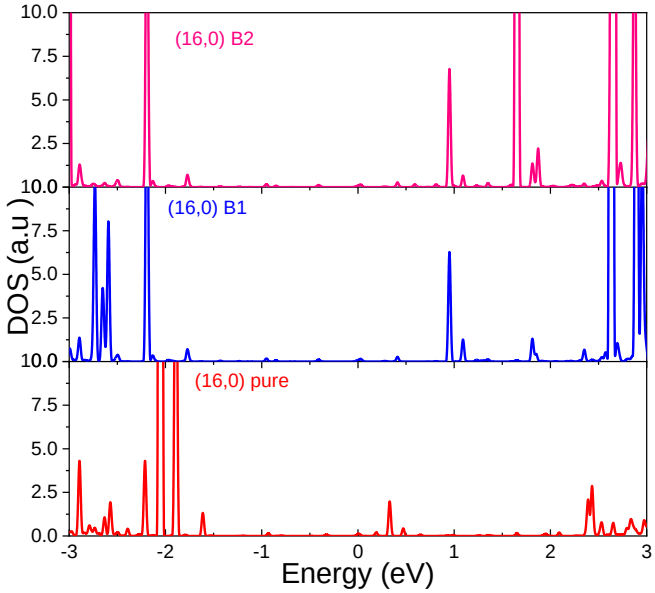

Figure 4 DOS of (n,0) for pure and N and B impurity states in 5 and 6 unit cell at (16, 0)

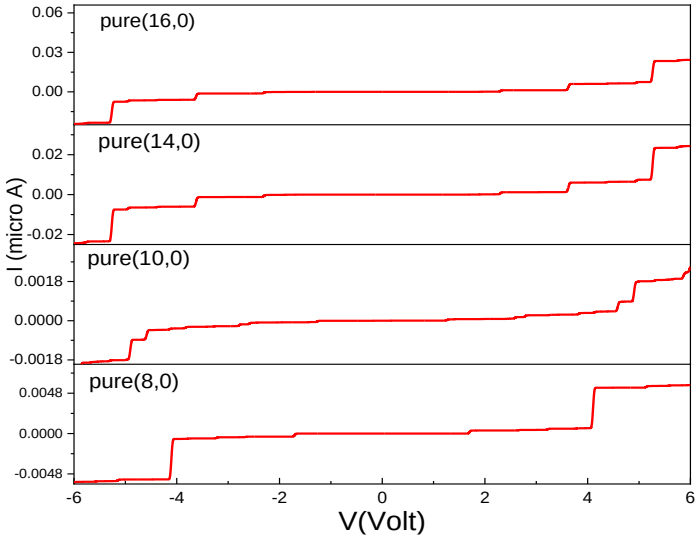

Figure 5 The current-voltage characteristics of the CNT/BN/CNT structure for n=6, 8, 14, and 16 in (n, 0) BCN nanotubes and (n, 0) CNTs, respectively.

The locations of the reservoir Fermi levels and the specifics of the wire's molecular structure dictate the places of the current jumps. An obvious characteristic of the molecular wire I-V curve is the development of jumps in the molecular eigenvalues.

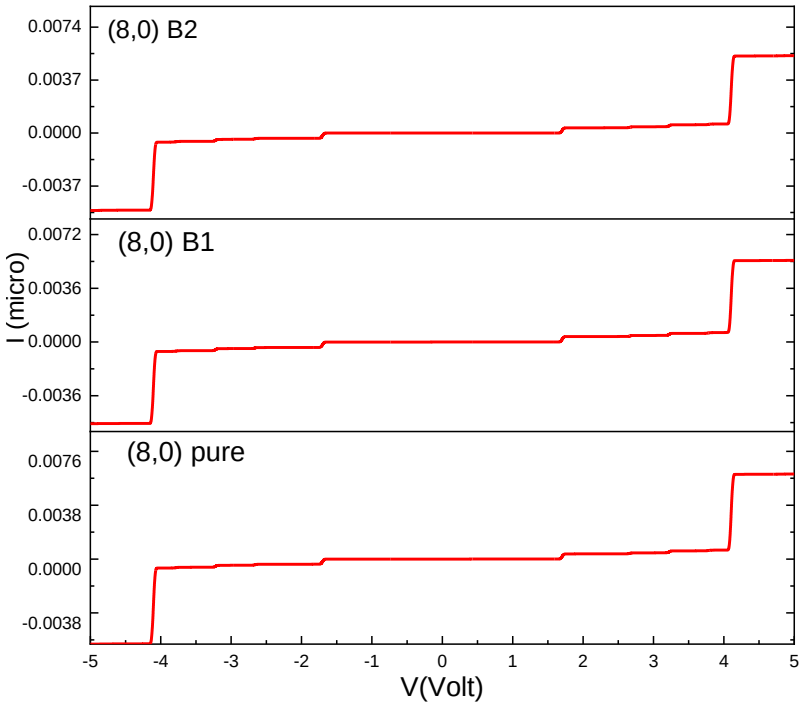

Figure 6 The current pure and after put impurity (B1,B2) at (n,0) for n=8 respectively

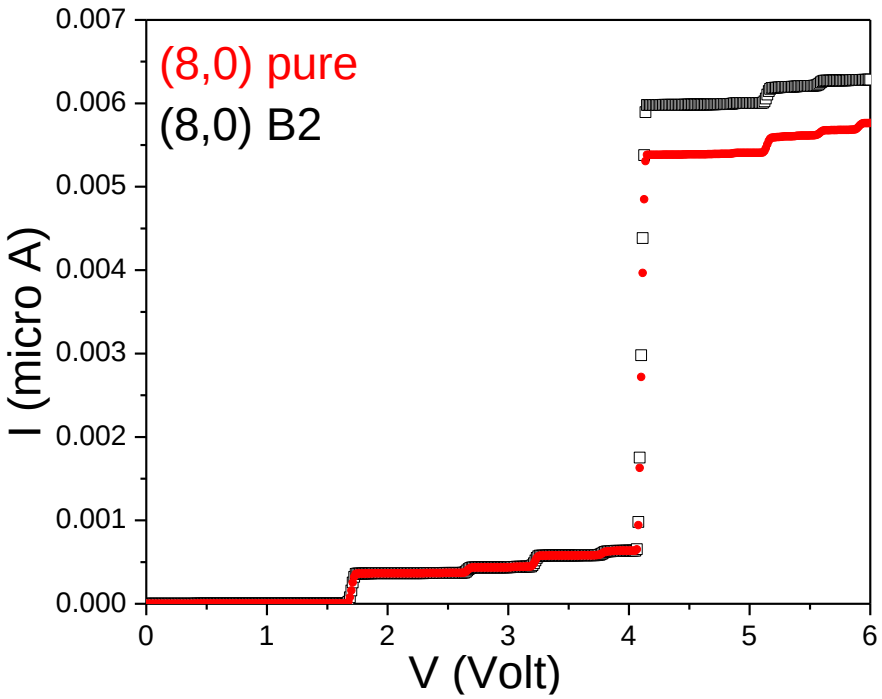

Figure 7 The poth current pure and after put impurity B2 at (8,0)

The two figures compare I-V values in the absence and presence of impurities, highlighting the influence of reservoir Fermi levels and wire structure on current jumps. This enables the development of a switching device.

Summary

We investigate the conductivity and I–V properties of zigzag (n, 0) single-walled BN nanotubes in a BN/CNT/BN structure using a tight binding model and some well-known methods. These approaches and methods are based on Green's function theory and Landauer formalism performed theoretically using MATLAB software. That nanocontacts is the n (n, 0) zigzag index of single-walled carbon nanotubes. We calculate the value of DOS in a tightly bound Hamiltonian way and compare it in three cases of index n (8, 0), (14, 0) and (16, 0). Our results indicate that B-doped and N-doped (n, 0) carbon nanotubes can be p- and n-type semiconductors, respectively.

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