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Theoretical study on the effect of dopant positions and dopant density on transport properties of a BN co-doped SiC nanotube

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ABSTRACT

We investigate the effect of dopant (boron 'B'–nitrogen 'N') position and density on electronic transport properties of a BN co-doped silicon carbide nanotube (SiCNT). The results show an increase in conductance when both BN impurities are far in space from each other. Orbital delocalization and appearance of new electronic states around Fermi level contribute to the current when this spacing is increased. On the other hand, a reduction in SiCNT conductivity was observed when BN dopant density was increased. This is attributed to the electronic states moving away from the Fermi level and orbital localization at higher bias voltages.

1. Introduction

Silicon carbide nanotubes have a great potential for application in chemical and biological sensors [1,2]. It is well known that bulk silicon carbide (SiC) is commonly contaminated by nitrogen and boron impurities where nitrogen substitutes the carbon site making n-type conductivity and boron substitutes both carbon and silicon sites forming an acceptor region in bulk SiC [3].

The electron transport properties of SiCNTs with individual boron and nitrogen doping have been reported in [2,4]. Hybridized connection of graphene and boron nitride nanoribbons is studied in [5]. The stability and electronic structures of boron–nitrogen and aluminium–phosphorus doped SiCNTs have been reported in [6,7]. Nitrogen doping-induced rectifying behavior in graphene nanoribbon devices were studied by [8]. Ferromagnetism induced by intrinsic defects and boron substitution in single-wall SiC nanotubes was reported by [9]. The transport properties, in presence of both boron and nitrogen impurities in SiCNT were recently investigated [10]. Here a silicon atom towards the left electrode was replaced by a boron atom forming a p-type (acceptor) region and a silicon atom towards the right electrode was replaced by a nitrogen atom making a n-type region. The dopant (BN) positions were arbitrarily fixed and the whole geometry was sought of as a p–n junction formed by a doped (8, 0) SiCNT placed between the gold (Au) electrodes [10].

The dopant position along the tube affects the electronic properties which have been observed previously for CNTs [11]. Therefore, it is of interest to find the effect of dopant (BN) positions on transport properties of a BN co-doped SiCNT, which has been investigated in this Letter. For this purpose, B and N impurities are adjusted (see Fig. 1) and then self consistent calculations are performed after relaxing the whole system using quasi-Newton optimization methods.

Because of their small feature size, it is difficult to study the transport properties of SiCNTs with traditional methods. In [4,10] and several other research works, electron transport properties have been successfully investigated using density functional theory (DFT) in combination with non-equilibrium Green's function (NEGF) formulation. In this Letter, we use DFT and NEGF to study the effect of dopant position on electron transport in BN co-doped SiCNTs. To the best of our knowledge, a similar kind of study (on the effect of BN dopant position and dopant density) has never been performed on BN co-doped SiCNTs.

2. Model and method

2.1. Simulation setup

To study the electron transport, a two probe geometry [4,10,12] that consists of a left semi-infinite electrode, right semi-infinite electrode and a central region (scattering region) was constructed using BN co-doped SiCNT and Au electrodes. Si–C bond length of 1.78 Å [4] and 1:1 Si–C ratio was considered. Both left and right electrodes are made up of 5 Au layers (in each of the *xyz* coordinates) perpendicular to the nanotube axis. Coupling gap between

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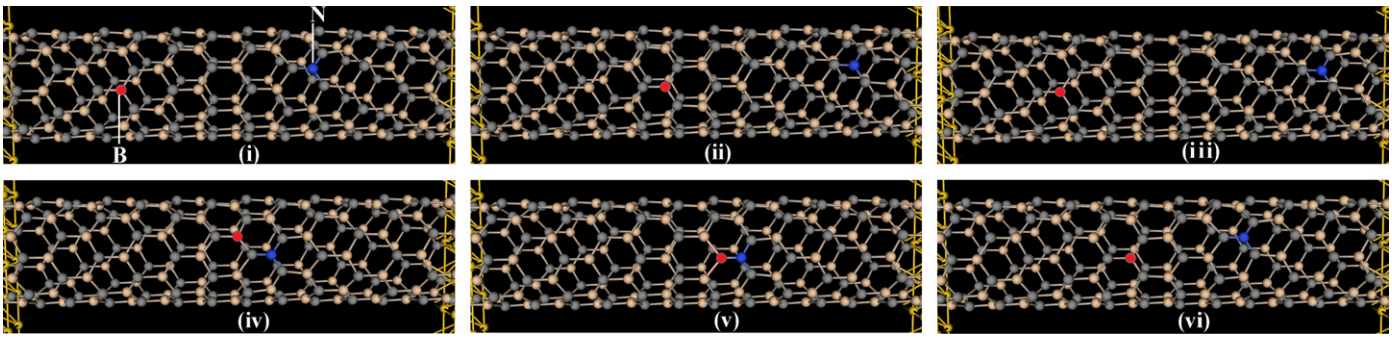

Fig. 1. Two-probe geometry of BN co-doped (8, 0) SiCNTs with Au electrodes. Dopant positions marked in red (boron) and blue (nitrogen) vary in (i)–(vi). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this Letter.)

the SiCNT and Au electrode is set as 1.3 Å which was found by relaxing a SiCNT and Au dimer (as reported in [10]).

The simulation parameters were selected as reported for CNTs in [12,13] and for SiCNTs in [3,4,10]. Mesh cut-off energy was 400 Ry, basis set was double zeta polarized with 0.001 Bohr radial sampling, exchange correlation functional was set to local density approximation (LDA) type with double zeta polarized (DZP) basis set, Brillouin zone integration parameters of three-dimensional electrodes are taken as (3, 3, 500). Self consistent calculations were performed on an *ab initio* based simulator called Atomistix [14] which uses density functional theory (DFT) and non-equilibrium Green's functions formulations (NEGF) together for obtaining electronic transport properties of molecules and devices. More details about the method and software could be found in previous reports [15–17]. Same simulator was used by [4] and several others for studying SiCNTs with individual boron and nitrogen doping.

The transmission spectrum describes the probability for electron with incident energy (E) to transfer from the left electrode to the right electrode under applied bias voltage (V). The analytical expression for calculating the transmission spectrum is given by [3,4,17] and were also used in our previous works [10,18], and hence are not repeated here again.

2.2. Geometry optimization of doped structures

Each BN doped structure shown in Fig. 1 was full relaxed before running simulations on them. After the introduction of BN impurities, doped SiCNT was relaxed using quasi-Newton geometry optimization methods until all residual forces on each atom are smaller than 0.05 eV/Å. A clearer picture of optimized structure is also shown below in Fig. 2, where bond lengths between the neighboring atoms of BN impurity are also shown. The bond length between boron and three carbon atoms, and the bond length between boron and three nitrogen atoms is in good agreement with other authors [3,19].

3. Electron transport on varying the B–N dopant spacing

3.1. Equilibrium transport properties with respect to the dopant position

The transmission spectrum $T(E)$ at various bias voltages is plotted in Fig. 3 corresponding to variations in dopant positions as shown in Fig. 1. Here the Fermi energy is set as 0 eV. The equilibrium transport properties (no bias voltage applied) of the BN-doped SiCNTs are studied firstly. A (8, 0) SiCNT is semiconducting by nature, a BN doped (8, 0) SiCNT is also semiconducting which is confirmed by the transmission gap (transmission coefficient is zero) around Fermi level in Fig. 3.

The highest occupied molecular orbital (HOMO) for structures (i), (ii), (iii), (iv), (v) and (vi) of Fig. 1 lie at −0.37 eV, −0.34 eV,

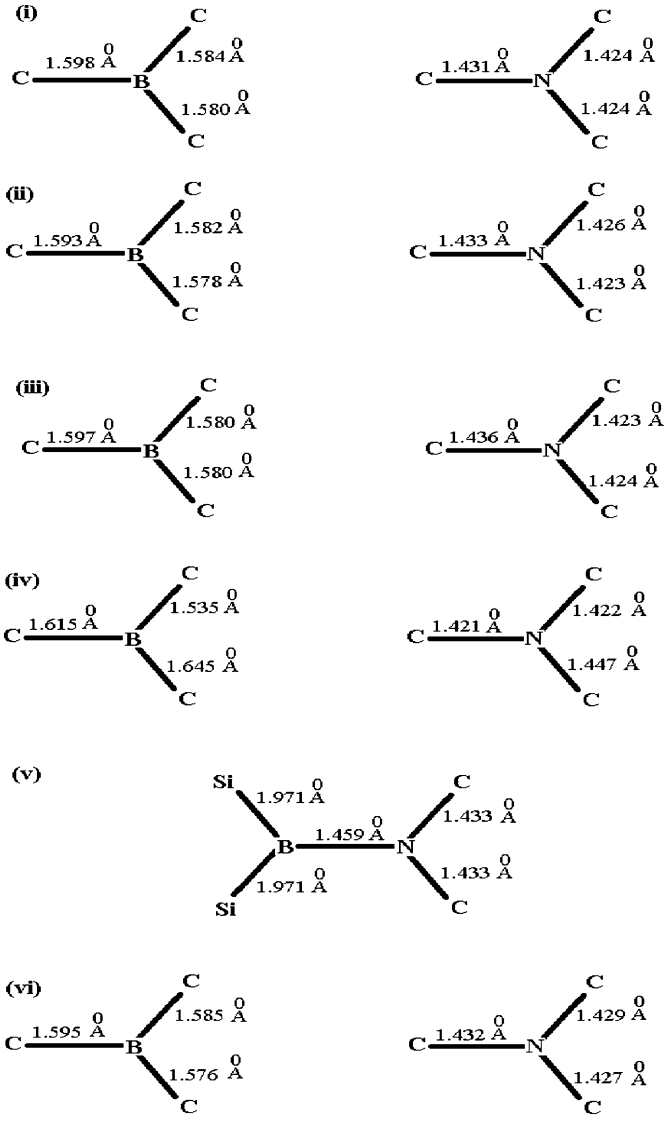

Fig. 2. Bond lengths (in Angstrom) between the neighboring atoms of boron and nitrogen dopants in SiCNT (obtained after full relaxation). Bonds shown in i–vi correspond to the structures shown in Fig. 1(i)–(vi).

−0.33 eV, −0.61 eV, −0.54 eV and −0.42 eV, it has no contribution from BN atoms. The lowest unoccupied molecular orbital (LUMO) for systems i, ii, iii, iv, v and vi of Fig. 1 lie at 0.17 eV, 0.19 eV, 0.15 eV, 0.43 eV, 0.18 eV and 0.23 eV, it is mainly contributed by N atom. HOMO–LUMO levels were obtained by observing the MPSH spectrum, the MPSH energies are shifted such that