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Electron transport properties of zigzag single walled tin carbide nanotubes

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ABSTRACT

A combined method of density functional theory and non-equilibrium Green's function formalism has been used to study the electron transport properties of zigzag single walled SnC nanotubes (SnCNTs) of different chiralities. Band structures of zigzag SnCNTs from (4,0) to (6,0) are calculated using $1 \times 1 \times 100$ *k*-point sampling. Transmission coefficients are computed for $(n,0)$ SnCNT ($n = 4,5,6$) devices at various positive and negative bias voltages within ±2.4 V. The current–voltage (*I–V*) curves in this bias voltage region show negative differential resistance (NDR), which is analyzed from the transmission spectra and molecular projected self-consistent Hamiltonian (MPSH) states. The rectifying performances of these devices are investigated by calculating the rectification ratio (I^+/I^-) with the bias voltage.

1. Introduction

The discovery of single walled carbon nanotubes (SW-CNTs) by Iijima [1], has made an explosion in their applications due to their unique structural and electronic properties. Devices like field-effect transistors, diodes, oscillators, switches, and chemical sensors have been designed and fabricated using SW-CNTs in recent years [2–6]. The unusual transport properties of nanodevices are known to be related with quantum phenomena. Some of these properties may be very sensitive to the atomistic changes in the system. An extensive review on the electron and spin transport in molecular devices has been made by Kim et al. [7]. The role of molecular orbitals in quantum transport through molecular devices and the effects of electric and magnetic fields on these molecular orbitals are discussed by Kim and Kim [8]. These authors have also highlighted the intuitive approach to design new electronic devices by appropriately tuning the molecular orbitals with external fields.

Nanotubes of hybrid atoms such as Si and C or Ge and C or Sn and C are also considered as important materials, which may be used as complementary to the conventional electronic devices. The physical and electronic properties of SiC, which is known to be a semiconductor with a wide band gap, have immense impact in the preparation of electronic devices used for high-temperature, high-power, and high-frequency applications [9]. Single walled SiC nanotubes (SW-SiCNTs) [10–12] are known to have better thermal stability, high chemical reactivity, and uniform semiconducting behavior independent of the chirality. Recently [13–15], SiCNTs are identified as promising biocompatible materials in various biomedical applications ranging from drug delivery and membrane separation to biosensors due to their higher solubility and less toxic effects than CNT itself in biological systems. Ketabi et al. [16] have carried out Monte Carlo simulation to study the complexes of DNA bases with Li doped SiCNTs in aqueous solutions. Hilder et al. [17] have investigated SiCNTs of various sizes as chloride-selective channels by performing classical molecular dynamics to examine the water and ion conductance through SiCNTs. Zhang et al. [18] have fabricated heterostructures of SW-CNTs and carbide nanorods based on controlled solid–solid reactions. Sun et al. [19] have prepared SiCNTs using the reaction of silicon obtained from a disproportion reaction of SiO with multiwalled CNTs. Transport properties of heterojunctions composed of SW-SiCNTs of different lengths coupled with SW-CNTs are theoretically studied recently [20] using a combined density functional theory (DFT) and non-equilibrium Green's function (NEGF) formalism. The characteristics of the current–voltage (*I–V*) curve of the SW-CNT/SW-SiCNT/SW-CNT heterojunctions are also investigated. Choudhary and Qureshi [21] have studied the effect of radial and axial deformation on electron transport properties of the semiconducting SiCNTs.

Being isoelectronic with C and Si, germanium compounds possess interesting characteristics, which are important for the nanoelectronics based technologies [22,23]. GeC in the bulk form is a semiconductor with a wide band gap and the percentage of covalency in GeC is comparable to that of SiC. Germanium filled carbon nanotubes with an average diameter of 15–100 nm are

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prepared by Domrachev et al. [24] by using metal–organic chemical vapor deposition (MOCVD) techniques. Electronic structures and geometries of three different types of armchair single walled GeC nanotubes (GeCNT) from (3,3) to (11,11) are calculated [25] using hybrid DFT and the finite cluster approximation. It is predicted that all armchair GeCNTs are semiconducting with a wide spectrum of band gaps ranging from 0.549 to 3.016 eV. Electronic and magnetic properties of semiconducting (8,8) SW-GeCNTs filled with iron nanowires are studied [26] using the first principle projector-augmented-wave (PAW) method within DFT under the generalized gradient approximation (GGA).

The element Sn being in the same group as C, Si, and Ge is expected to show some importance in nanotechnology. Saha et al. [27] have successfully prepared Pt/SnC NW/carbon paper composite electrodes, which show higher specific electrochemical surface area and enhanced tolerance to CO than that of the commercial Pt/C electrode. Recently [28], Sn-filled multiwalled carbon nanotubes are prepared by using metal–organic CVD and their electromagnetic absorption properties are determined. Wu et al. [29] have synthesized the carbon coated SnO_2 nanotubes, which are applied as anode materials for lithium–ion batteries. Şahin et al. [30] using plane-wave DFT method and phonon-mode calculations have predicted that binary compounds of group-IV elements like SiC, GeC, SnC, SnSi, SnGe, and SiGe have stable honeycomb structures. Among these, SiC, GeC, and SnC are planar like graphene, while all other compounds are buckled for stabilization. The nanotubes consisting of Sn and C are expected to draw attention to the researchers to mimic the nanodevices and search for their potential applications in biological systems as observed in graphene [31] and graphene-like materials [32]. Lü et al. [33] have performed first principle calculations based on DFT and the quasiparticle GW approximation to study the electronic properties of mono layered planar honeycomb structured SiC, GeC, and SnC nanosheets and compared to those of graphene. The GeC nanosheet possesses a direct band gap at the k point, while both SiC and SnC have indirect band gaps. The conduction band minimum for SnC has been predicted to be at the Γ point. The band structures of these nanosheets can be controlled by elongating or reducing the bond length. The strained nanosheets have some potential applications in optoelectronics and energy engineering. Following the observation of the band structure of SnC nanosheet, we urge to investigate the electronic properties of zigzag SnCNTs and devices. The present study explores hitherto unknown electron transport properties of $(n,0)$ SnCNT for $n = 4$–6 by using a combined DFT and NEGF formalism. Transmission energy spectrum, band structure, and density of states (DOS) are determined. The I–V characteristics and rectification ratio (I^+/I^-) of (4,0), (5,0), and (6,0) SnCNT devices are also studied under different bias voltages.

2. Method of computation

In order to study the electron transport properties of $(n,0)$ SnCNTs, we have adopted a two-probe model which consists of a left electrode (L), right electrode (R), and a central region (C). Atoms in both the electrodes include parts of the semi-infinite bulk electrodes, which interact with the atoms of the central region. The contact dependency is minimized by using SnCNT electrodes similar to the central region in the two-probe model [21]. In the present study, the coupling effect as well as length dependency are neglected by keeping a minimal length segment (10 Å) of SnCNT in the central region. Geometries of the perfect $(n,0)$ SnCNTs are optimized first, and then the optimized structures are used to construct the two-probe model. The composite nanodevices thus obtained, are further relaxed. The quantum transport calculations of the optimized devices are carried out using ATK package [34], which is based on the combination of DFT and Keldysh NEGF method [35,36]. The double-ζ polarized (DZP) basis sets for both Sn and C along with the norm conserving Troullier–Martins pseudopotentials [37] are used in the present calculations. The exchange correlation potential is approximated by the Perdew–Burke–Ernzerhof (PBE) parameterization [38] of GGA function. The electrostatic potentials are computed on a real-space grid with a mesh cutoff energy of 150 Ry. The electrode temperature has been set to 300 K and the $1 \times 1 \times 100$ k-point sampling is employed throughout the calculation. The zero biased total energy and transmission spectra are calculated with $1 \times 1 \times 500$ and $1 \times 1 \times 1000$ k-point samplings. However, no appreciable changes are found in the total energy and transmission spectra upon the variation in k-point sampling in the transport direction (z-direction) and the $1 \times 1 \times 100$ k-point sampling has been found to be good enough.

Within the NEGF formalism, the current (I) that passes through the central region (C) at a finite bias voltage (V_b) can be computed using Landauer–Büttiker formula [39]:

$$I(V_b) = \frac{2e}{h}\int_{\mu_L}^{\mu_R} T(E,V_b)[f(E,\mu_L) - f(E,\mu_R)]dE, \quad (1)$$

where f is the Fermi function, $\mu_{L,R}$ are chemical potentials of the left and right electrodes, respectively and $T(E,V_b)$ is the transmission coefficient at energy E and bias voltage V_b. The transmission coefficient, which determines the probability of electrons transferring between the two semi-infinite electrodes, can be evaluated by following equation:

$$T(E,V_b) = Tr[\Gamma_L(E,V_b)G(E,V_b)\Gamma_R(E,V_b)G^{\dagger}(E,V_b)], \quad (2)$$

where $G(E,V_b)$ is the Green's function of the two-probe model and $\Gamma_{L/R}$ are the coupling matrices.

3. Results and discussion

Geometries of SW-SnCNT devices of chiralities (4,0)–(6,0) are optimized at the PBE/DZP level of theory using $1 \times 1 \times 100$ k-point sampling. Fig. 1 shows the optimized structure of the (6,0) SnCNT device. The Sn–C bond length in the ground state ($^3\Pi$) of diatomic SnC molecule has been calculated to be 2.02 Å using multireference configuration interaction calculations [40]. In zigzag SnCNTs, each Sn atom is bonded to two symmetrically equivalent carbon atoms with a shorter bond length, while the third Sn–C bond is longer by 0.02–0.04 Å. A different hybridization of Sn and C compared to pure CNT results in some distortions in the C–Sn–C and Sn–C–Sn bond angles, which vary between 106° and 121°.

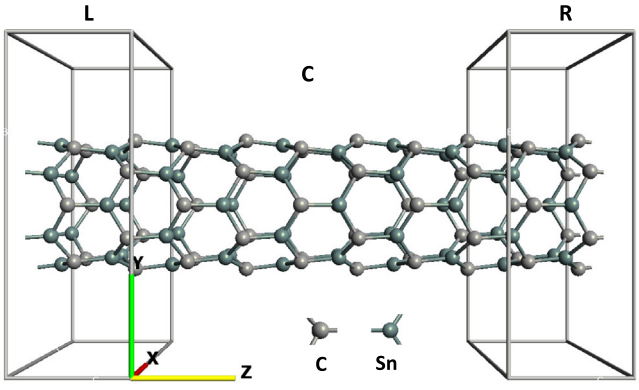

Fig. 1. Optimized geometry of (6,0) SnCNT device at the PBE/DZP level of theory using $1 \times 1 \times 100$ k-point sampling.