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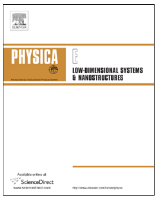

Tuning the electronic properties of single-walled SiC nanotubes by external electric field

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ABSTRACT

The electronic properties of SiC nanotubes (SiCNTs) under external transverse electric field were investigated using density functional theory. The pristine SiCNTs were semiconductors with band-gaps of 2.03, 2.17 and 2.25 eV for (6,6), (8,8) and (10,10) SiCNTs, respectively. It was found the band gaps was reduced with the external transverse electric filed applied. The (8,8) and (10,10) SiCNTs changed from semiconductor to metals as the intensity of electric field reached 0.7 and 0.5 V/Å. The results indicate that the electronic properties of SiCNTs can be tuned by the transvers electric field with integrality of the nanotubes.

1. Introduction

Since the carbon nanotubes (CNTs) were found in 1991 by Iijima [1], which have aroused much interest in the nanotechnology field [2–6] due to their unique physical and chemical properties, such as superconducting, good mechanical properties, light weight and flexibility. Based on the above properties, CNTs are expected to be applied in electronic nano-devices. Other nanotubular structures, such as BN, AlN, and CdS nanotubes [3,6–8] have also been synthesized to study the size effect of nanomaterials and their potential applications in nano-devices. Most of the current semiconductor technologies are based on silicon materials, scientists endeavor to synthesize Si-based nanotubes and graphene-like sheets to reduce the size of the electronic devices based on Si-related materials, however, it is very difficult to fabricate stable Si nanotubes and graphene-like Si sheets since the hybridation orbit of Si and C was different, and Si prefers sp^3 instead of sp^2 hybridization [9,10]. There is a possible way to build stable Si nanotubes by mixing Si and C atoms. SiC Nanotubes (SiCNTs) have been successfully synthesized in 2001 by shape memory synthesis method [11]. The SiCNTs have many advantages over the CNTs because of their high reactivity of their exterior surface and specific surface. The SiCNTs can be used as an excellent sensor for detecting toxic gas, such as CO, HCN, NO, and HCOH [11–13]. Also the SiCNTs can adsorb more hydrogen atoms than pure CNTs, so SiCNTs are promising materials for hydrogen storage [14]. These properties of SiCNTs are not sensitive to their chirality, but they dependents on the diameter size.

The atomistic structures of single-walled SiCNTs had been investigated by *ab*-initio method [15]. Theoretical results indicate that the Si and C atoms are arranged alternately to form a hexagonal structure, the hexagon is composed of three Si atoms and three C atoms. SiCNTs show semiconductor characteristics with a wide band-gap, which shows less dependence on the helicity, but which increases with the increase of the diameter of the SiCNTs [10,16,17]. For a practical application of SiCNTs in electronic devices, it is better to control the electronic properties of SiCNTs as required. Doping is a common method to tune the electronic properties of semiconductors. The band gap of SiCNTs can be tuned through doping with other atoms, such as adsorption of K, N, and H atoms [18–22], however, doping will lead to a significant changes of the geometric configuration and shift the Fermi energy to valence band or conduction band [20,23,24]. Other methods, such as strain [25] or introducing defects [26,27], also can be used to tune the electronic properties of SiCNTs. However, the strain and defects are not easy to be controlled experimentally.

In this paper, we investigated the electronic properties of SiCNTs under external transverse electric field using spin-polarized density functional theory (DFT) calculations. Results show the electronic properties of SiCNTs can be tuned by the transvers electric field.

2. Computational details

All of these calculations were performed by first principles

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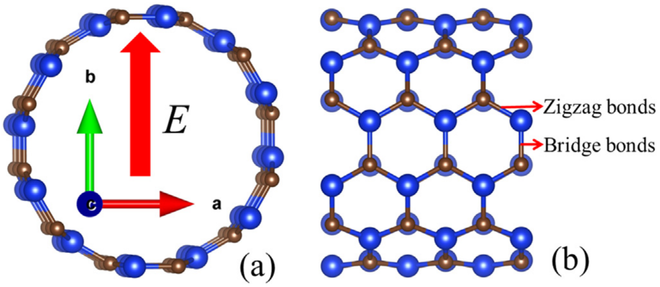

Fig. 1. Cross-sectional view of (a) (6,6) SiCNTs, brown and blue balls represent carbon and silicon atoms, respectively. The red arrow indicates the direction of external transverse electric field (*E*). (b) Side view of (6,6) SiCNTs marked zigzag bands and bridge bands.

based on the spin DFT within SIESTA code [28] which adopted the generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) to describe the electron-exchange correlation [29–31]. Norm-conserving pseudopotentials [32] were adopted to describe electron-ion interaction. And the valence electron wave functions were expanded using a double-ζ basis set plus polarization functions. A $1\times1\times9$ Monkhorst-Pack mesh for the *k*-points sampling of the Brillouin zone integration was used. Three armchair (6,6), (8,8) and (10,10) SiCNTs were modeled to calculate electronic structures with an external electric field, and the SiCNTs were consisting of 72, 96 and 120 atoms for (6,6), (8,8) and (10,10) SiCNTs, respectively, with Si-to-C ratio of 1:1. Geometry structures of single-walled SiCNTs are fully optimized until the atomic forces on each atom are less than 0.02 eV/Å.

3. Results and discussion

To avoid periodic image interaction between the SiCNTs, the SiCNTs were put into a box with $a=b=70$ Å, $c=9.33$ Å. *a* and *b* were kept constant, whereas *c* is free to relax upon geometry optimization until the atomic forces are less than 0.02 eV/Å on each atom. Cross-sectional and side-views of the relaxed atomic configurations of (6,6) SiCNTs are shown in Fig. 1(a) and (b), respectively. The calculated bond lengths are 1.798 Å for the zigzag bonds and 1.796 Å for the bridge ones, which agrees well with the previous reported range from 1.79–1.80 Å [33–35].

Fig. 2(a) shows the band structure of (6,6) SiCNT, which has an indirect band gap with valence band maximum (VBM) at Γ point and conduction band minimum (CBM) located at *Z* point. (8,8) and (10,10) SiCNTs shows the same characters, as shown in Fig. 2(e) for (8,8) SiCNTs. The calculated band-gaps are 2.03, 2.17 and 2.25 eV for (6,6), (8,8) and (10,10) SiCNTs, respectively. The band gap increases with the increase of diameters, which agrees with previous reports [17,36,37]. SiCNTs with larger diameter have wider band gap because the hybridization effect is weak for larger-diameter SiCNTs [38], and the smaller-diameter SiCNTs have a narrow band-gap for the σ–π orbitals rehybridization caused by the high curvature [39].

Evolution of the band structures of (6,6) SiCNT under external electric field is shown in Fig. 2(b–d), the external transverse electric field is applied along *b*-axis as shown in Fig. 1(a). It can be seen from Fig. 2 that the band-gap decreases with the increasing the external electric field. The (6,6) SiCNT preserved the indirect band gap semiconductor character with VBM located in Γ point and CBM located in *Z* point as the external electric field applied. The band gaps are 1.47, 0.64, and 0.19 eV for the (6,6) SiCNT with external electric field of 0.4, 0.8, and 1.0 V/Å, respectively. The evolution of the band structures of (8,8) SiCNTs under external electric field shows the same characters as shows in Fig. 2(f–h). The reason leading to this result is asymmetry of electrostatic potential under the electric field applied. The charge density of lowest state of the conduction band is moved along the opposite direction of the applied electric field, and the charge density of highest state of the valence band is moved along the direction of the applied electric field [36,40]. The energy of CBM state shifts down due to the charge accumulated in regions of higher electrical

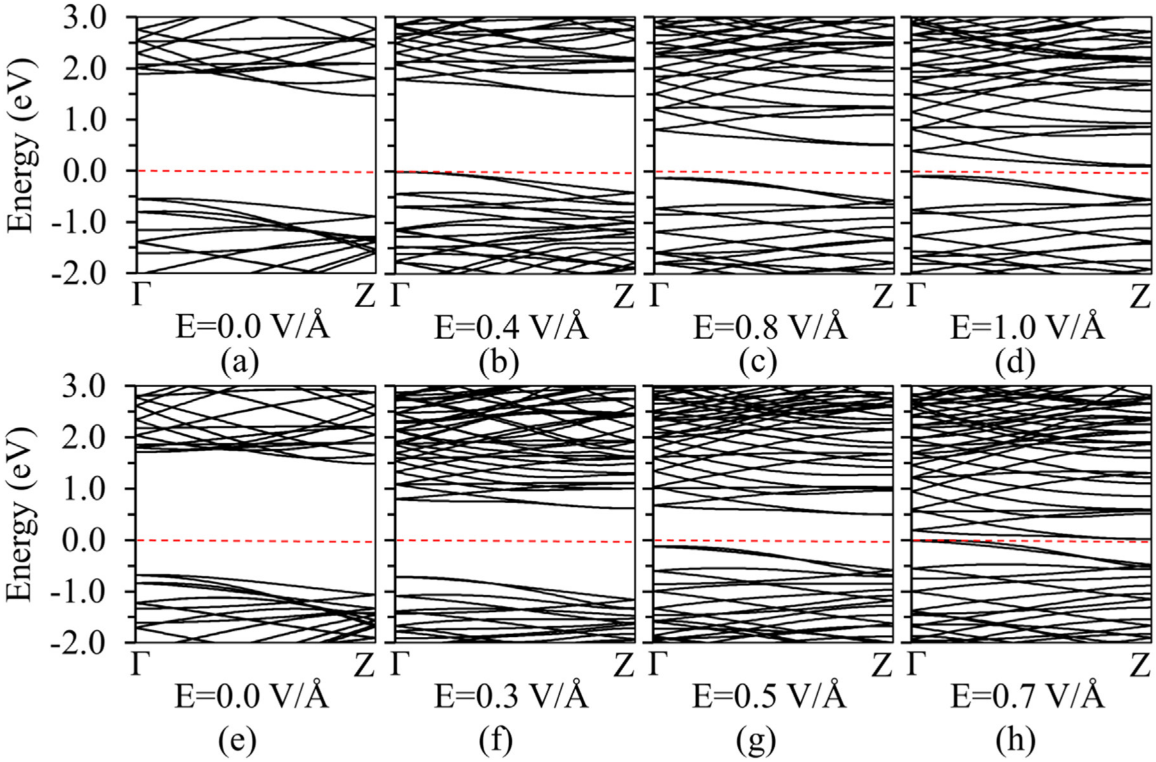

Fig. 2. Electric band structures for (a–d) (6,6) SiCNTs and (e–h) (8,8) SiCNTs under different electric field. Red dash lines represent Fermi level which was set to be zero.