

# Effects of inter-tube coupling on the electro-optical properties of silicon carbide nanotube bundles studied by density functional theory



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## ARTICLE INFO

### Article history:

Received 2 May 2015

Received in revised form 13 June 2015

Accepted 15 June 2015

Available online 19 June 2015

### Keywords:

Density functional theory

SiCNT

Electronic structure

Optical properties

## ABSTRACT

The electronic and optical properties of bundled armchair and zigzag silicon carbide nanotubes (SiCNTs) are investigated by using density functional theory. The effects of inter-tube coupling on the electronic dispersions of SiCNT bundles are demonstrated. It was found that the band structure of (6,0) SiCNT bundle shows metallic feature. The calculated dielectric functions of the armchair and zigzag bundles are similar to that of the isolated tubes, except for the appearance of broadened peaks, small shifts of peak positions about 0.1 eV and increasing of peak intensities. For (6,0) SiCNT with smaller radius, by considering interband and interband transitions, the band structure coupling causes an extra peak at low energies.

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## 1. Introduction

Since the discovery of carbon nanotubes (CNTs) by Iijima [1], an extensive research field in the nanoscale opened due to their exceptional electronic, mechanical, thermal and optical properties. Carbon nanotubes exist in several forms from individual single-walled and multi-walled tubes to carbon nanotube bundles. CNTs can be considered as a layer of graphene sheet rolled up into a cylinder [2], and the structure of a CNT is completely specified by the chiral vector which is given in terms of a pair of integers ( $n, m$ ). CNTs can be chiral or nonchiral depending on the way they are rolled up. Their physical properties, in particular, optical dielectric functions, depend sensitively on their chirality, i.e., the ( $n, m$ ) indices [3]. Apart from CNTs, inorganic tubular materials, such as BN [4], AlN [5], GaN [6], have also been predicted and synthesized. These tubular materials also display some very interesting properties distinctly different from their bulks. Bulk silicon carbide (SiC) is a suitable material for electronic devices for high-temperature, high-power, and high-frequency applications, due to its unique physical properties [7]. Silicon carbide nanotubes (SiCNTs) were also synthesized via the reaction of CNTs and SiO at different temperatures [8]. The structure and stability of SiC nanotubes have been investigated using ab initio density functional theory in detail [9–11]. It was found that the SiC nanotubes with alternating Si–C bonds are more stable than the forms which contain C–C or Si–Si bonds [9]. While CNTs have been found to be either metallic or semiconducting depending on their diameter and chirality, these

calculations show that all the SiCNTs are semiconductors. The energy band gap of the SiCNTs is dependent on their diameter and chirality, with direct gaps for zigzag tubes and indirect gaps for armchair and chiral tubes [9,10]. This is due to the difference in the electronegativity of Si and C atoms, leading to the ionicity of Si–C bonds in the SiCNTs which localizes the electronic states. Carbon nanotubes are highly aromatic systems. Replacing one half of the C atoms in CNTs by Si atoms decreases the aromaticity of each six-membered ring. The decreasing of aromaticity leads to the decreasing of stability. Therefore, the exterior surface of SiCNTs has a higher reactivity with respect to the SWCNTs. For example, the electronic structures of SiCNTs can be manipulated by selected hydrogenation [12], and SiH<sub>3</sub> and CH<sub>3</sub> radicals can also be chemically adsorbed on the SiC nanotubes to form acceptor or donor levels depending on the adsorption sites [13]. In addition, the electrical and magnetical properties of SiCNTs can be tuned by appropriate doping [14–18]. Recently, a series of ab initio calculations have been carried out to analyze the linear optical features and underlying band structure of all three types of the SiCNTs as well as their possible dependence on diameter and chirality [19,20]. Electronic and optical properties may change significantly when nanotubes are bundled together [21,22]. Kozinsky and Marzri [23] studied the static dielectric properties of isolated single-walled and multi-walled CNTs and nanotube bundles by density functional perturbation theory. For single-walled CNTs the longitudinal polarizability is proportional to the inverse square of the band gap and the transverse polarizability is proportional to the inverse square of the effective radius. For the case of bundled nanotubes, the longitudinal polarizabilities are the same as those

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of isolated nanotubes and the transverse polarizabilities depend strongly on the tube–tube distance of the bundles. Using Rayleigh scattering spectroscopy, Wang et al. [24] investigated the optical transition of given individual CNTs in their isolated and bundled form. They concluded that the bundling effects produce a red shift of optical transitions due to the mutual dielectric screening of CNTs in a bundle. In this article, for the first time, we investigate the electronic, and optical properties of armchair [(4,4), (5,5), (6,6)] and zigzag [(6,0), (8,0), (9,0)] silicon carbide nanotube bundles using density functional theory calculations.

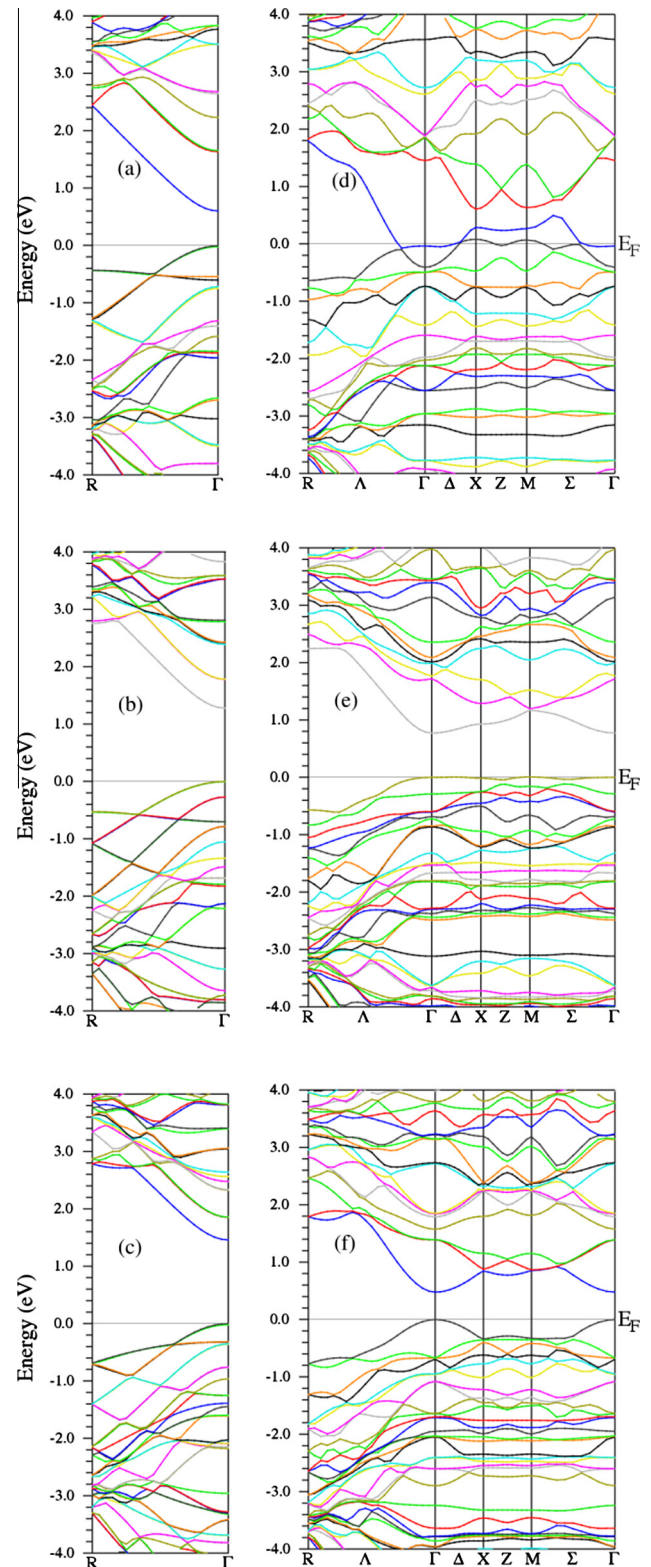
In Section 2 computational model and method are presented. Section 3 contains results and discussion. Final section is conclusion.

## 2. Computational model and method

The total energy and electronic band structure calculations are performed via first principles full potential linearized augmented plane-wave density functional theory, as implemented in the WIEN2K code [25]. In order to achieve energy eigenvalues convergence, the wave functional in the interstitial region was expanded in terms of plane waves with a cut-off parameter of  $RMT \times K_{max} = 7$ , where RMT denotes the smallest atomic sphere radius and  $K_{max}$  is largest  $k$  vector in the plane wave expansion. DFT has proven to be quite successful and in quantitative agreement with experimental data for sp<sup>2</sup>-like materials, especially graphite [26–28]. For investigation of the interaction between bundles, the density functional is treated by the local-density approximation (LDA) with the exchange and correlation potential parameterized by perdue and wang, [29]. The core states are the 1s electrons of C atom and up to 2p for Si atom. Muffin-tin radii are 1.3 and 1.85 au for C and Si atoms, respectively. The optimizations were carried out with respect to both the atomic coordinates and the lattice constants, using PORT method (a reverse-communication trust-region Quasi-Newton method form the Port library). Structural optimizations are converged when the forces acting on each atom were smaller than 0.01 eV/Å. The optical spectra were calculated using 300 k-points in the first Brillouin zone and broadening for optical spectra is set to 0.1 eV.

## 3. Results and discussion

The equilibrium inter-tube separation distances determined by total energy optimization are 3.40, 3.48 and 3.51 Å for the zigzag (6,0), (8,0) and (9,0) bundles, respectively and 3.58, 3.54 and 3.53 Å for the armchair (4,4), (5,5) and (6,6) bundles, respectively [30]. Here we will focus on the description of the effects of tube–tube interaction on the electronic and optical properties of SiCNT bundles. In Figs. 1 and 2, we present the band structure of the selected zigzag and armchair SiCNT bundles along the high-symmetry directions in the hexagonal Brillouin zone. The electronic band structures along the tube axis for the corresponding isolated tubes are also presented for comparison. The electronic band structures of the isolated (6,0), (8,0) and (9,0) SiCNTs indicate that these zigzag SiCNTs have a direct band gap at the  $\Gamma$  point. This suggests that the zigzag SiCNTs may find applications in optical and optoelectronic devices such as SiC lasers. The calculated band gap is 0.62, 1.15 and 1.40 eV for (6,0), (8,0) and (9,0) SiCNTs, respectively, which is in agreement with other ab initio results [19,20]. In contrast, armchair SiCNTs are indirect band-gap semiconductors (see Fig. 2). For the armchair SiCNTs, the bottom of the conduction bands generally appears at the 1D Brillouin zone boundary, while the top of the valence bands occurs at somewhere between the 1D Brillouin zone boundary points (Fig. 2). The calculated band gap is 1.60, 2.07 and 2.11 eV for (4,4), (5,5) and (6,6)



**Fig. 1.** Band structure of: isolated (a) (6,0), (b) (8,0) and (c) (9,0) SiCNT along the tube axis, (d) (6,0), (e) (8,0) and (f) (9,0) SiCNT bundle along the high symmetry directions of the first Brillouin zone.

SiCNTs, respectively, which is consistent with the previous calculational case [19,20]. After analyzing in detail and comparing the band structures of isolated zigzag and armchair SiCNTs [Figs. 1(a)–(c) and 2(a)–(c)] and their bundled counterparts [Figs. 1(d)–(f) and 2(d)–(f)] along the tube axis, we summarize

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