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Modulation of electronic properties of silicon carbide nanotubes via sulphur-doping: An *ab initio* study

Ram Sevak Singh [a,*], Ankit Solanki [b]

[a] Department of Physics, National Institute of Technology, Kurukshetra 136119, Haryana, India
[b] School of Material Science and Nanotechnology, National Institute of Technology, Kurukshetra 136119, Haryana, India

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ABSTRACT

Silicon carbide nanotubes (SiCNTs) have received a great deal of scientific and commercial interest due to their intriguing properties that include high temperature stability and electronic properties. For their efficient and widespread applications, tuning of electronic properties of SiCNTs is an attractive study. In this article, electronic properties of sulphur doped (S-doped) zigzag (9, 0) SiCNT is investigated by *ab initio* calculations based on density functional theory (DFT). Energy band structures and density of states of fully optimized undoped and doped structures with varying dopant concentration are calculated. S-doped on C-site of the nanotube exhibits a monotonic reduction of energy gap with increase in dopant concentration, and the nanotube transforms from semiconductor to metal at high dopant concentration. In case of S-doped on Si-site doping has less influence on modulating electronic structures, which results in reduction of energy gap up to a moderate doping concentration. Importantly, S preferential substitutes of Si-sites and the nanotube with S-doped on Si-site are energetically more stable as compared to the nanotube with S-doped on C-site. The study of tunable electronic properties in S-doped SiCNT may have potential in fabricating nanoelectronic devices, hydrogen storage and gas sensing applications.

1. Introduction

Discovery of carbon nanotubes (CNTs) has opened an avenue towards theoretical and experimental study of various non-carbon nanostructures that include boron nitride, silicon carbide nanotubes (BNNTs and SiCNTs) [1–5]. Behaving as metal or semiconductor with narrow band gap, CNTs have received much interest wordwide due to their fascinating properties and great potential for scientific and technological applications. However, electronic properties of carbon nanotubes are strongly dependent on the chirality of the nanotube, and it is challenging task to control precisely both chirality and diameter during the synthesis process. Non-metal nanotubes that include BNNTs and SiCNTs, on the other hand, are not sensitive to chiral characteristics. Therefore apart from CNTs, SiCNTs have been predicted and synthesized [1,6–9]. Bulk SiC, a wide band gap semiconductor, has been widely utilized in the area of high temperature, high frequency, high voltage and large power that are attributed to its wide band gap, highly saturated electron mobility, high breakdown field strength, high thermal conductivity and radiation resistance [10,11]. Compared to bulk SiC the tubular form of SiC also exhibits many interesting properties that include large surface, underscoring its potential in sensing and many other applications in nanoelectronics [12,13]. Unlike CNTs, SiCNTs are polar materials with Si–C bond length (1.771 Å) much larger than C–C bond length (1.42 Å) in CNTs [9]. Because of these structural differences, SiCNTs exhibit many physical properties distinctively different from CNTs. For example, SiCNTs have high thermal stability, lower strain energy and large band gap which is directly or indirectly depending on the chirality of the nanotubes [9]. In addition, larger bond length in SiCNTs make them a more appropriate candidate for applications in hydrogen storage [14]. Experimental and theoretical methods have been employed to study the electronic and structural properties of undoped and doped SiCNTs [15]. Gali et al. studied electronic structure of B and N doped SiCNTs using first principle calculations [13]. Alam et al. applied a density functional theory to study zigzag SiC nanotubes [16]. Using theoretical approaches it is predicted that SiCNTs are a better candidate for hydrogen storage and doping scheme can further be applied to enhance the storage capacity [14,17,18]. As such research works in this area are ongoing. Systematic theoretical and experimental studies on alteration of electronic properties of SiCNTs via appropriate dopants are needed to explore the possibility of its utilization in scientific and commercial applications. In this article, we have first time investigated the electronic properties evolution in a zigzag (9, 0)

* Corresponding author.
E-mail address: singh915@gmail.com (R.S. Singh).

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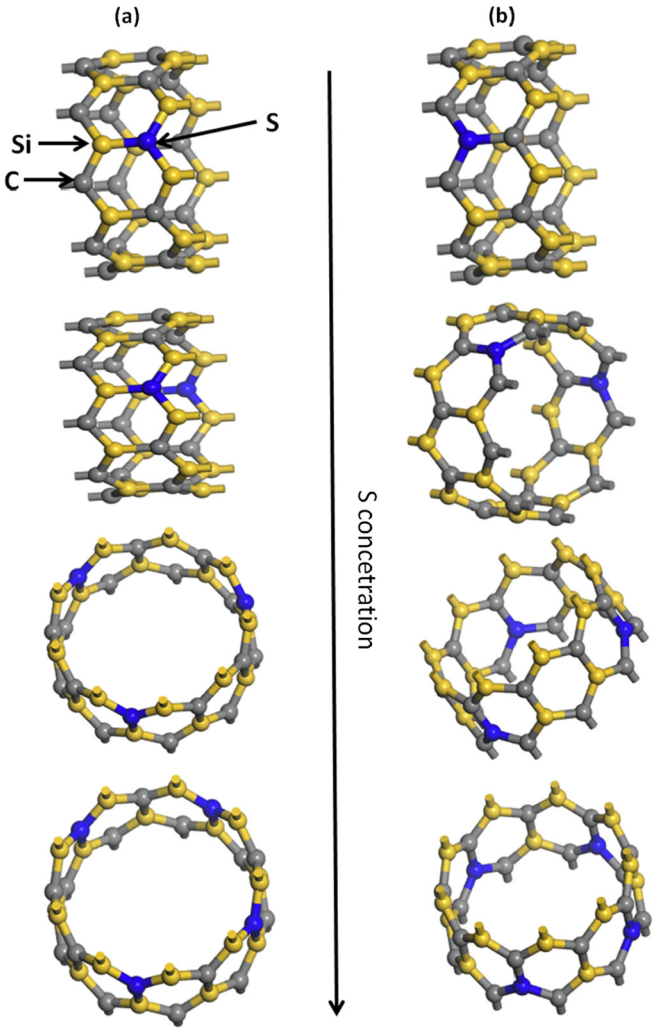

Fig. 1. Nanostructures of S-doped zigzag (9, 0) SiCNTs. (a) S-doped on C-site with increasing S concentration (top to bottom). (b) S-doped on Si-site with increasing S concentration (top to bottom). S atom is indicated by blue color. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

SiCNT via a systematic S-doping scheme. Electronic band structures and density of states of all optimized structures are calculated using first principle calculations based on density functional theory (DFT). The presented results of electronic band structures and density of states have been obtained by performing calculations using plane wave pseudo-potential technique based on density functional theory with CASTEP module of Materials Studio 7. The plane wave cut-off energy is set to 320 eV and the exchange correlation effects are described by generalized gradient approximation (GGA) [19]. All atomic geometry optimizations were performed in the first Brillouin zone using k-points generated by a uniform $1 \times 1 \times 8$ grid parameters. Using the ultrasoft pseudopotentials [20] all the geometries were optimized until the force on each atom is less than 0.05 eV/Å. The Si–C bond length in SiCNT were chosen to be 1.771 Å, and diameter of zigzag (9, 0) nanotube to be 8.79 Å.

2. Results and discussion

2.1. Structural properties of S-doped SiCNTs

Nanotube structures and position of dopants are depicted in Fig. 1. S atoms were substituted on C- and Si-sites of the nanotubes with increasing S concentration. Structural properties of doped

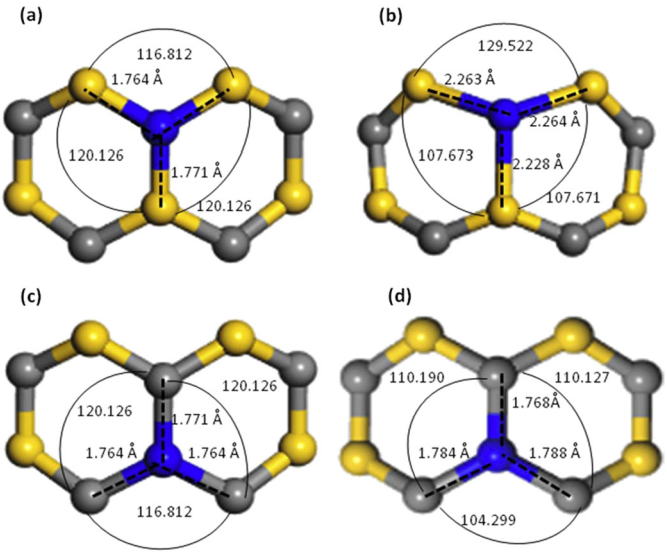

Fig. 2. (a) The structure of S-substituted on C-site before optimization. (b) The structure of S-substituted on C-site after optimization. (c) The structure of S-substituted on Si-site before optimization. (d) The structure of S-substituted on Si-site after optimization.

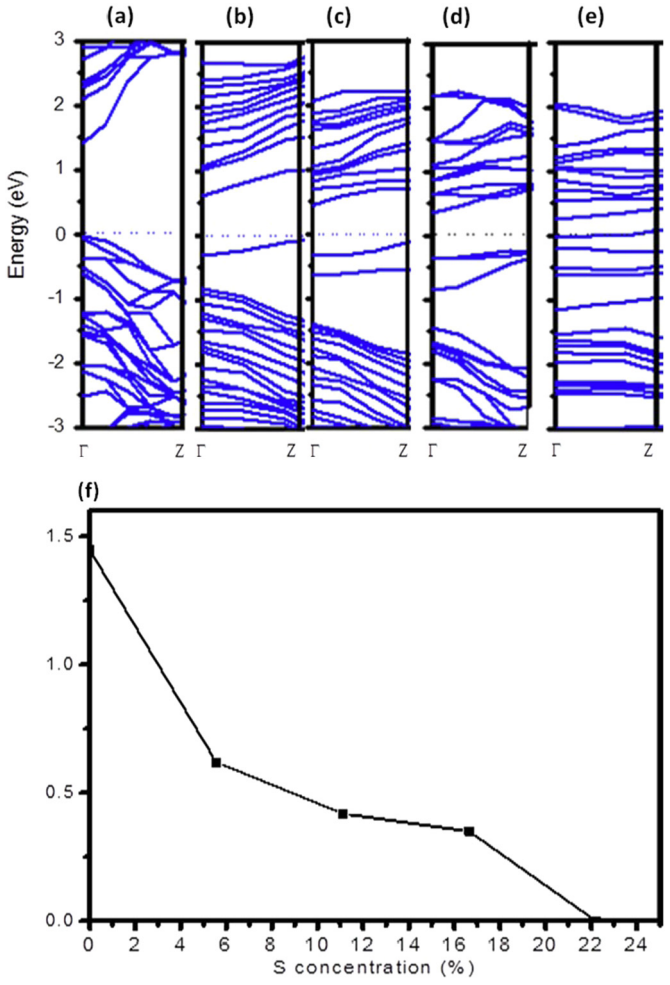

Fig. 3. Electronic properties of S-doped on C-site of SiCNTs. (a) Band structure of undoped SiCNT, (b)–(e) S-doped SiCNTs with increasing dopant concentration, and (f) Band gap vs. S concentration. Fermi level is set to zero and presented by dotted line.