



Electronic structures of Stone–Wales defective chiral (6,2) silicon carbide nanotubes: First-principles calculations



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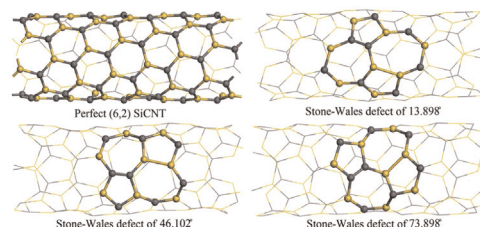
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HIGHLIGHTS

- Geometries of Stone–Wales defects in the chiral (6,2) SiCNT are investigated.
- Formation energies of the Stone–Wales defects are sensitive to their orientation.
- High similarity in electronic structures of Stone–Wales defective SiCNTs is found.
- Differences in properties of defective SiCNTs can be improved by electric fields.

GRAPHICAL ABSTRACT

Geometries of Stone–Wales defects with different orientations in a (6,2) silicon carbide nanotube and their impacts on the electronic structures of the nanotube are investigated with first-principle calculations.



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ABSTRACT

By using first-principle calculations based on density functional theory, the geometries and electronic structures of the Stone–Wales defective chiral (6,2) silicon carbide nanotubes (SiCNTs) are investigated. Independent on their orientations, Stone–Wales defects form two asymmetric pentagons and heptagons coupled in pairs (5–7–7–5) and a defect energy level in the band gap of the SiCNT. By applying transverse electric fields, significant differences in the electronic structures of the defective (6,2) SiCNTs are achieved, which may provide the foundation of identifying the orientation of Stone–Wales defects in chiral SiCNTs.

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1. Introduction

Because of their unique properties and potential applications in preparation of electronic devices and sensors working in high power and high temperature environment [1–3], silicon carbide nanotubes (SiCNTs) have attracted tremendous interests. With substitution reactions between silicon atoms and multi-walled

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carbon nanotubes (CNTs), SiCNTs are synthesized for the first time [4]. The radio-frequency magnetron sputtering method, the hydrothermal method and the chemical vapor deposition (CVD) method are also successfully applied to prepare SiCNTs [5–7]. Although the qualities of the synthesized SiCNTs have been improved significantly, the experiment conductions in above processes (such as sputtering and high temperature) often lead to point defects, especially native defects. The influences of vacancies and antisite defects on the electronic properties of SiCNTs have been predicted with theoretical calculations [8–10].

Stone–Wales defect is a typical defect in nanotubes materials.

The impacts of this defect on the properties of the CNTs and boron nitride nanotubes (BNNTs) are extensively studied. The band gap of the zigzag (10,0) CNT is narrowed obviously by the Stone–Wales defect [11]. Partovi-Azar's studies indicate that the influences of the defects in CNTs seriously depend on their orientations and the circumferential defect can even lead to a (semi) metal–semiconductor transition in armchair CNTs [12]. Stone–Wales defects may form one or two defect energy levels in the band gap of zigzag BNNTs, which is determined by the diameter of the BNNT [13,14]. More important, Wang's studies indicate that Stone–Wales defects in SiCNTs can be caused by irradiation [15]. Independent on the orientations of the defects, they form two defect energy levels in the band gap of the armchair (5,5) SiCNT [16]. Due to the complexity in modeling and calculations on the chiral SiCNTs, these nanotubes are rarely studied [17]. Until now, no investigations on the Stone–Wales defective chiral SiCNTs are reported.

In this work, the impacts of Stone–Wales defects on the (6,2) SiCNT are investigated with first-principle calculations based on density functional theory (DFT), which has been successfully applied in studies on the perfect and doped SiCNTs [18–25]. The influences of the Stone–Wales defects on the geometry of the SiCNT are obtained by analysis of the variations of the nanotube in the defect regions. Furthermore, the electronic structures of the Stone–Wales defective (6,2) SiCNTs are calculated, particularly the band structures of the defective SiCNTs under transverse electric fields. These researches are helpful for identifying the orientation of the Stone–Wales defect in chiral SiCNTs.

2. Computational methods

Under the reference of Alfieri's investigations on chiral SiCNTs [17], the model for the (6,2) SiCNT is established (in Fig. 1(a)). The diameter of the nanotube is about 7.12 Å. This model is placed in the center of a hexagonal supercell. The supercell length in the lateral direction is 30 Å to eliminate the interaction between the adjacent images, and the length in the axial direction is 19.25 Å, which is the same as the length of the nanotube. To release the stress in the model and obtain the structure similar to the prepared nanotube, geometry optimization on the (6,2) SiCNT is realized. The convergence criteria are determined by the energy, stress and displacement of each atom, which are set as less than 1×10^{-4} Ha, 0.02 Ha/Å and 5×10^{-3} Å. Lengths of the Si–C bonds in the optimized SiCNT vary in the range from 1.780 Å to 1.793 Å.

In a nanotube with given radius and chiral angle (r and χ ,

respectively), the Stone–Wales defects have three possible orientations of χ , $\pi/3 - \chi$ and $\pi/3 + \chi$ [26]. The orientations angle θ of a Stone–Wales defect can be described by its direction of the short axis and the rolling direction of the SiC layer similar to graphene. The chiral angle of the (6,2) SiCNT is 13.898°. Stone–Wales defects with orientation angles of 13.898°, 46.102° and 73.898° are shown in Fig. 1(b), (c) and (d). These models can be established by rotating the C–Si₁ bond, C–Si₂ bond and C–Si₃ bond in Fig. 1(a).

The electronic structures of the perfect and defective (6,2) SiCNTs are calculated by means of all-electron linear combination of atomic orbital density functional theory implemented in DMol³ package [27]. The exchange-correlation potential is realized with the generalized gradient approximation (GGA) provided by Perdew, Burke and Ernzerhof (PBE) [28]. Double numerical plus d -function is used as atomic orbital basis set throughout the calculations. The Brillouin zone sampling is performed using special k points generated by the Monkhorst–Pack grid with a value of $1 \times 1 \times 8$, which is suitable to one dimensional material [29].

3. Results and discussion

3.1. Electronic structures of the perfect (6,2) SiCNT

To analyze the impacts of the Stone–Wales defects, the electronic structures of the perfect (6,2) SiCNT are calculated. (6,2) SiCNT has an indirect band gap of 1.456 eV. The bottom of the conduction band for the nanotube locates at the Z point of the first Brillouin zone, and the top of the valence band lies at the point T labeled out in Fig. 2 (a). The conduction band mainly consists of Si 3p states (Fig. 2 (b)). The upper valence band is mainly originated from C 2p states and Si 3p states. The lower valence band is formed primarily with C 2s states and Si 3s states. The bottom of the conduction band and the top of the valence band are occupied by Si 3p states and C 2p states. The distributions of the partial density of states (PDOS) for the (6,2) SiCNT are similar to those of Si and C atoms in the (9,0) SiCNT [30].

3.2. Local structures of Stone–Wales defects

Formation energy is defined as the required energy to form a Stone–Wales defect in a SiCNT and can be calculated as

$$E_{form} = E_{defective} - E_{perfect} \quad (1)$$

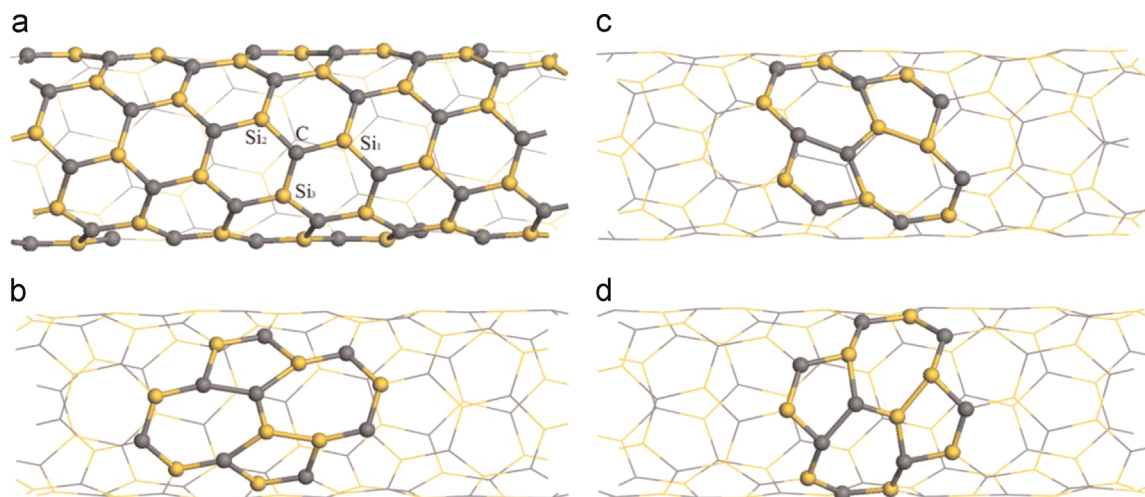


Fig. 1. Models for perfect (a) and Stone–Wales defective (6,2) SiCNTs, the orientation angles of the Stone–Wales defects are 13.898°(b), 46.102°(c) and 73.898°(d). Yellow and gray balls indicate Si and C atoms. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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