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The electronic properties of chiral silicon nanotubes

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ABSTRACT

This paper investigated the geometric structural and electronic properties of infinite chiral single- and doubel-walled silicon nanotubes (SWSiNTs and DWSiNTs) using density functional theory (DFT). With the periodic boundary conditions (PBC), the structures of infinite chiral silicon nanotubes (SiNTs) were obtained and their electronic properties were discussed in detail. The stability of the chiral SWSiNTs was enhanced with the increase of the diameter. For the chiral DWSiNTs, with the increase of the wall spacing, the stability of chiral DWSiNTs (n,n/2)@(2n,n) was gradually enhanced but the chiral DWSiNTs (2n,n)@(3n,3n/2) was reduced; and with the increase of the diameter, the stability of chiral DWSiNTs was gradually enhanced. And the chiral SWSiNTs (n,m) showed semiconductor properties when the chiral indexs were not multiple of 3; otherwise, they exhibited metal characteristics. The electronic properties of SWSiNTs (4,2) and (6,3) were abnormal due to the curvature effect. For chiral DWSiNTs, the orderliness of band gaps was the same as SWSiNTs. In other words, when the chiral indexs for two tubes were both multiple of 3, they show metal characteristics. When the chiral indexs of just one tube were not multiple of 3, they exhibited semiconductors properties, except for (4,2)@(8,4) which showed metal characteristics due to the curvature effect.

1. Introduction

With the discovery of carbon nanotubes (CNTs) [1] and the synthesis of the very uniform single-walled carbon nanotubes (SWCNTs) [2,3], more and more scientists are devoted to the field of nano materials. Although silicon and carbon elements belong to the same group in the periodic table, the silicon atom is larger than the carbon atom. One of the distinctive features of the silicon atom is that it can generate various stages of the sp^2 or sp^3 hybrid formation, such as silicon clusters [4], silicon nanoparticles [5], silicon nanowires [6–9] as well as SiNTs [10,11]. SiNTs have a wide range of applications in the field of nano electronic devices such as transistors, sensors, field emitting devices, nano magnetic devices and optoelectronic devices. Sha J. et al. [12] have reported that SiNTs with diameters ranging from 50 nm to 100 nm were prepared by chemical vapor deposition (CVD) as template, which provided the material basis for the further study of the properties and applications of SiNTs.

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In recent years, a number of experimental researchers have tried to develop the synthesis of SiNTs through a lot of methods such as template combined process [12,13], template combined molecular beam epitaxy process [14], electrochemical deposition process [15], hydrothermal process [16,17], dc-arc plasma process [18,19], other CVD process [20], dual RF plasma process [21] as well as removable template [22–24]. Although great progresses have been made in experimental researches, the theoretical research is still in the weak link, mainly focusing on the effect of doping other elements on the structure of SiNTs. Many theoretical researchers have tried to develop the SiNTs by the first-principles method or the molecular dynamics method. For instance, Zhang et al. [25] investigated the possible structures of zigzag SWSiNTs; Zhao et al. [26] discussed several structures of zigzag DWSiNTs; M. Taghinejad et al. [27] studied the evolution of SiNTs; Chen et al. [28] researched the existence and stability of the armchair DWSiNTs; Zhu [29] et al. reported the coronal multi-walled SiNTs; Liu [30] et al. considered the electronic properties of armchair SWSiNTs and DWSiNTs; and Lin [31] et al. probed the electronic properties of zigzag SWSiNTs and DWSiNTs. However, there has not yet been any researched been reported on chiral SiNTs. Therefore, it is necessary to explore the chiral SiNTs. In this paper, we explore the geometric structural and electronic properties of chiral SWSiNTs and DWSiNTs via the first-principles method based on DFT, which can help to predict the properties of chiral SiNTs.

2. Methods

In this paper, the exchange-correlation potential energy function is expressed by un-restricted B3LYP [32,33]. In particular, the 3–21 g [34,35] basis sets were chosen since it has been used to describe the geometric structure features and electronic properties of chiral CNTs [36] and is more accurate than the LANL2DZ basis sets which has been used to describe the geometric structure features and electronic properties of armchair SiNTs [30] and zigzag SiNTs [31]. Although 6–31 g basis sets are more accurate than 3–21 g basis sets, the calculated silicon bond length is 0.2389 nm and 0.2395 nm respectively, but they are coincide with the experimental results (0.2246 nm) within the error range [37]. In order to improve efficiency, we chosen 3–21 g basis group.

Firstly, using imposing periodic boundary conditions (PBC) [38] and choosing B3LYP function with 3–21G basis set, the repeated units to obtain the infinite chiral SiNTs and optimize it. Secondly, the energy band structures are described based on the 240 k-points and 10 energy levels which are selected up and down around the Fermi level. Finally, the densities of states (DOS) are calculated by wave functions of output coefficient matrix and their discrete peaks are broadened with a parameter of 0.3eV by using Gaussian functions.

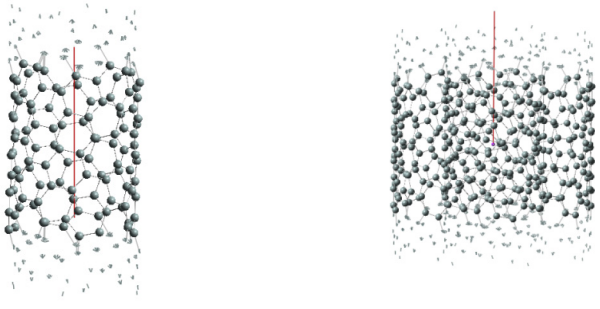
All of the above calculations are carried out with Gaussian 03 program package [39].

3. Results and discussion

In this paper, we explored the infinite chiral SWSiNTs (n,n/2) (n = 4,6,8,10,12,14,16,18,20) and infinite chiral DWSiNTs (n,n/2)@(2n,n) (n = 4,6,8,10) and (2n,n)@(3n,3n/2) (n = 4,6).

3.1. Structural stability

Fig. 1 shows the optimized geometric structures of SiNTs. To analyze the stabilities of these optimized geometric structures of SiNTs, we calculated the average binding energy (E_b). The average binding energy is defined as the energy gained during assembling tubular clusters from isolated silicon atoms. It can be calculated by



(a) (b)

Fig. 1. (a) The optimized geometric structures of the infinite SWSiNT (8,4) and (b) DWSiNT (8, 4)@(16, 8).

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