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Theoretical studies on the electronic structures and spectra of single silicon-doped SWCNTs

Research Article

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Abstract: The equilibrium geometries and electronic structures of a series of SWCNTs doped with a silicon atom were studied by using density function theory (DFT). The most stable doping site of silicon predicted at B3LYP/6-31G(d,p) level was located near the boundary of the SWCNTs. The energy gaps of (3,3) C_{48}, (3,3) C_{60} and (3,3) C_{72} were respectively decreased by 0.43, 0.25 and 0.14 eV after doping. Based on the B3LYP/6-31G(d) optimized geometries, the electronic spectra of the doped SWCNTs were computed using the INDO/CIS method. The first UV absorption at 973.9 nm of (5,5)-Si(L) ($C_{59}Si$) compared with that at 937.5 nm of (5,5) (C_{60}) was red-shifted. The ^{13}C NMR spectra and nuclear independent chemical shifts (NICS) of the doped SWCNTs were investigated at B3LYP/6-31G(d) level. The chemical shift at 119.4 of the carbon atom bonded with the silicon atom in (3,3)-Si(L) ($C_{59}Si$) in comparison with that at 144.1 of the same carbon atom in (3,3) (C_{60}) moved upfield. The tendency of the aromaticity (NICS = -0.1) for (3,3)-Si(H) ($C_{47}Si$) with respect to that of the anti-aromaticity (NICS = 6.0) for (3,3) (C_{48}) was predicted.

Keywords: *Si-doped SWCNTs • Stability • NMR spectra• Aromaticity • DFT*

1. Introduction

Nano materials have been widely studied [1-2] since they have extraordinary magnetic [3] and optical properties [4]. The discovery of carbon nanotubes [5] is a milestone in the research of nano science and technology. The preparation and modification of single-walled carbon nanotubes (SWCNTs) are carried out because of the unique electronic and mechanical characteristics. Many attempts have been made to synthesize the SWCNTs, including the use of arc plasma [6] and chemical vapor deposition (CVD) [7-8]. On one hand, unmodified SWCNTs exhibit some amazing characteristics such as the duality of the semi-conductivity and conductivity [9]. This duality depends on the diameter of the SWCNTs and arrangement of the hexagons [10]. Besides the electrical conductivities, a tunable optical property of the SWCNTs has been observed in Jeffrey's experiments [11]. In addition, the dispersed SWCNTs have also played an important role in the enhancement of the effective thermal conductivity of fluids [12]. On the other hand, the chemical modification on the SWCNTs is an effective way in altering the physical and chemical properties of the SWCNTs. The SWCNTs doped with boron and nitrogen are beneficial to promoting the chemisorption of transition-metals on the SWCNTs [13]. The massive SWCNTs doped with nitrogen and phosphor are also promising in preparing nano diodes [14]. Silicon has a similar electronic attribute to carbon. Thus the doping of silicon may be friendly to the pristine SWCNTs, which brings new properties without breaking the innate structure and stability.

Song *et al*. found that the stiffness of the SWCNTs could be decreased by the doping of silicon using the molecular dynamics [15]. Rahmandoust and Öchsner also studied the mechanical property of the Si-doped SWCNTs and drew the similar conclusion in a finite and elementary model [16]. However, there was no report on the electronic properties of the Si-doped SWCNTs. Based on the above consideration, the electronic structures of the single silicon-doped SWCNTs with definite lengths were investigated. Then the comparison between the pristine and doped SWCNTs was made. Finally, the dependence of the properties for the SWCNTs on the size was explored.

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2. Theoretical Method

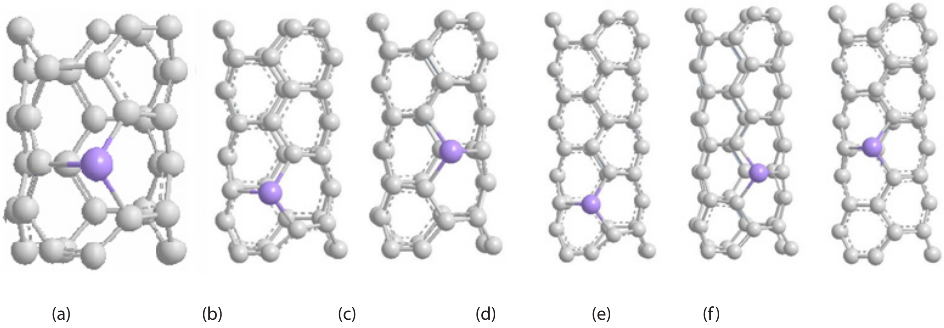
In this article, the SWCNTs with the definite lengths were used. Triple bonds between the carbon atoms without hydrogen atoms were formed on the boundary. The SWCNTs were modified by replacing one carbon atom with a silicon atom, and only the carbon atoms away from the boundary were considered. For the definite-length SWCNT (3,3) (C_{36}), there was only one kind of doping site, and (3,3)-Si(L) ($C_{35}Si$) was designed, shown in Scheme 1 (a). (4,4)-Si(L) ($C_{47}Si$), (5,5)-Si(L) ($C_{59}Si$) and (6,6)-Si(L) ($C_{71}Si$) with the increasing radii were formed at the same doping site as that of (3,3)-Si(L) ($C_{35}Si$). As the lengths of the SWCNTs increased, more possible doping sites appeared. Scheme 1 (b) and (c) illustrated the two possible configurations of (3,3)-Si ($C_{47}Si$), which were denoted as (3,3)-Si(L) ($C_{47}Si$) and (3,3)-Si(H) ($C_{47}Si$). Analogously, the three possible configurations of (3,3)-Si ($C_{59}Si$) were denoted as (3,3)-Si(L) ($C_{59}Si$), (3,3)-Si(M) ($C_{59}Si$) and (3,3)-Si(H) ($C_{59}Si$) shown in Scheme 1 (d), (e) and (f), respectively.

Full geometric optimization without any symmetric restriction for the SWCNTs was performed using AM1 method [17]. Further optimization of these SWCNTs was carried out employing Becke three parameters plus Lee, Yang and Parr's (B3LYP) method [18-20] with 6-31G(d) basis set in DFT. The equilibrium geometries with the minimum energies of the SWCNTs were obtained. The energies at the single point of the SWCNTs were computed at B3LYP/6-31G(d,p) level. These methods in Gaussian 03 program [21] have been used in the investigation on the electronic structures of the supra-molecular complexes [22-24], hydrogen-bonding systems [25,26], conductive polymers [27], fullerenes [28-33], carbon nanotubes [34] and other compounds [35-40]. Based on the optimized geometries at B3LYP/6-31G(d) level, the electronic spectra of the SWCNTs were calculated by using the configuration interaction (CI) method. The INDO/CIS model was implemented as in the INDO program improved by Zerner (ZINDO [41]) without any adjustment of parameters. The ^{13}C NMR spectra of the SWCNTs were calculated with the gauge-independent atomic orbital (GIAO) at B3LYP/6-31G(d) level. This method had been used in studying the NMR spectra of organic compounds such as cyclopropenyl acetylenes [42], barbituric acid [43] and alloxan-based thiosemicarbazones [44]. The difference in the chemical shifts between the individual helium atom and helium atom inside the SWCNT was defined as the NICS value. A helium atom was used as a mass center of the geometry for the SWCNT optimized at B3LYP/6-31G(d) level. The NICS values at the tube center of the SWCNTs were studied on the GIAO method at B3LYP/6-31G(d) level. The NICS values had been used as a reliable criterion of aromaticity, which was proposed by Schleyer *et al.* [45-49].

3. Results and Discussion

3.1. Stability of the doped SWCNTs

The lengths of C-C bonds in (3,3) (C_{36}) was 1.500 Å, which was basically in agreement with the reported values 1.420 Å [9] and 1.430 Å [13]. The low distortion energy of the doped SWCNTs led to the high stability. The relative energy of (3,3)-Si(L) ($C_{47}Si$) was lower than that of (3,3)-Si(H) ($C_{47}Si$) (Table 1). Thus (3,3)-Si(L) ($C_{47}Si$) was more stable than (3,3)-Si(H) ($C_{47}Si$), which was related to the distortion energy caused by the Si-C bonds. In (3,3)-Si(L) ($C_{47}Si$) (L-configuration), the lengths of the Si-C bonds were 1.807, 1.824 and 1.904 Å, respectively. In (3,3)-Si(H) ($C_{47}Si$), the lengths of the Si-C bonds were 1.856, 1.868 and 1.940 Å. The shorter Si-C bonds in (3,3)-Si(L) ($C_{47}Si$) led to a weaker structural strain. A low distortion energy was stored in (3,3)-Si(L) ($C_{47}Si$). Similarly, (3,3)-Si(L) ($C_{59}Si$) compared with (3,3)-Si(M) ($C_{59}Si$) or (3,3)-Si(H) ($C_{59}Si$) exhibited the low relative energy. The lengths of the Si-C bonds in (3,3)-Si(L) ($C_{59}Si$) were 1.800, 1.805 and 1.867 Å, the lengths of the Si-C bonds in (3,3)-Si(M) ($C_{59}Si$) were 1.852, 1.855 and 1.945 Å, and those in (3,3)-Si(H) ($C_{59}Si$) were 1.857,



Scheme 1. The configurations of (a) (3,3)-Si(L) ($C_{35}Si$), (b) (3,3)-Si(L) ($C_{47}Si$), (c) (3,3)-Si(H) ($C_{47}Si$), (d) (3,3)-Si(L) ($C_{59}Si$), (e) (3,3)-Si(M) ($C_{59}Si$) and (f) (3,3)-Si(H) ($C_{59}Si$)

Table 1. Relative energy of doped (3,3) SWCNTs at B3LYP/6-31G(d,p) level

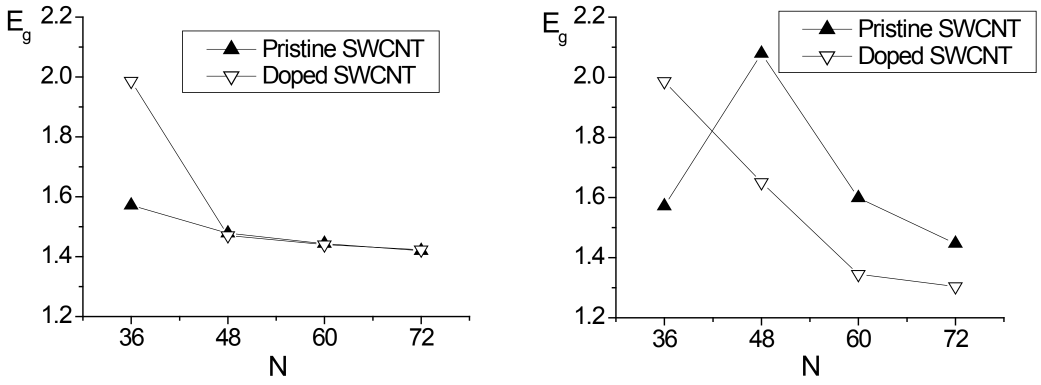
SWCNTs	Relative Energy (kJ mol^{-1})	SWCNTs	Relative Energy (kJ mol^{-1})
(3,3)-Si(L) ($C_{47}Si$)	0	(3,3)-Si(L) ($C_{59}Si$)	0
(3,3)-Si(H) ($C_{47}Si$)	68.5	(3,3)-Si(M) ($C_{59}Si$)	73.1
		(3,3)-Si(H) ($C_{59}Si$)	39.9

1.868 and 1.965 Å. (3,3)-Si(L) ($C_{59}Si$) had the shortest Si-C bonds and the lowest distortion energy, thus it was the most stable configuration of the three configurations. It could be predicted that the L-configuration would still be stable if the lengths of the SWCNTs were elongated to (3,3) (C_{72}) or (3,3) (C_{84}).

3.2. Electronic structures at the ground state

The energy gaps of SWCNTs could be changed with the change in the radii or lengths. On one hand, the increase in the radii of the SWCNTs led to the decrease in the energy gaps (Fig. 1a). The overlapping of the electron cloud between the sp²-C atoms was improved owing to the good planarity of the SWCNTs with the large radii. Compared with those of the pristine SWCNTs, the energy gaps of (4,4) $C_{47}Si$, (5,5) $C_{59}Si$ and (6,6) $C_{71}Si$ were basically unchanged. Only (3,3) C_{36} exhibited the increased energy gap after doping, which could be relevant to its small size both in the radius and in the length. On the other hand, the increase in the lengths of the pristine SWCNTs resulted in an oscillation regularity of the energy gaps (Fig. 1b). The energy gap of (3,3) (C_{72}) was 1.45 eV, which was basically consistent with the experimental value 1.1 eV [50]. The energy gaps of the pristine SWCNTs would continue to oscillate if the lengths were further increased. This oscillation had been observed in Lu's study on SWCNTs [51]. However, in the doped SWCNTs, the oscillating dependence of the energy gaps on the lengths disappeared. This doping effect was promising in manufacturing the length-tunable electronic device in the future. Compared with those of the pristine SWCNTs, the energy gaps of (3,3) $C_{47}Si$, (3,3) $C_{59}Si$ and (3,3) $C_{71}Si$ were decreased. It was reported that the energy gaps of the SWCNTs doped with N and P atoms were reduced in comparison with those of the parent SWCNTs as well [14], supporting our conclusion.

The doping site of the silicon atom also affected the energy gap of the SWCNT. (3,3)-Si(L) ($C_{47}Si$) possessed the narrower energy gap of 1.65 eV than that of 1.87 eV for (3,3)-Si(H) ($C_{47}Si$). Likewise, the energy gap 1.34 eV of (3,3)-Si(L) ($C_{59}Si$) was narrower than 1.52 eV of (3,3)-Si(H) ($C_{59}Si$). The L-configurations were lowly symmetric, while the H-configurations were highly symmetric. The splitting of the energy levels arising from the low symmetry lessened the energy gap of the L-configuration.



(a) (b)

Figure 1. Dependence of the energy gaps (E_g) at B3LYP/6-31G(d,p) level on the total number (N) of atoms in the SWCNTs, N was increased by (a) Radial enlargement and (b) Elongation in length

3.3. Electronic absorption spectra

The electronic states of the SWCNTs were changed upon the doping of the silicon atom, which affected the absorptions in the electronic spectra of the SWCNTs. The first absorption peak of (4,4) (C_{48}) was located at 977.8 nm, and that of (5,5) (C_{60}) was at 937.5 nm. It had been observed in the experiment that the first absorption peak of (6,5) SWCNT was near 990 nm [11], which supported our calculation results. On one hand, the first absorptions for most of the doped SWCNTs compared with those of the pristine SWCNTs were red-shifted (Table 2). This resulted from the reduced energy gaps of the doped SWCNTs. On the other hand, the first peaks of L-configurations compared with those of the other configurations were also red-shifted. For example, the first absorption at 880.9 nm of (3,3)-Si(L) (C_{47}Si) with respect to that at 737.3 nm of (3,3)-Si(H) (C_{47}Si) was red-shifted. Similar red-shift in the first peak at 1056.2 nm of (3,3)-Si(L) (C_{59}Si) relative to that at 894.4 nm of (3,3)-Si(M) (C_{59}Si) or 766.8 nm of (3,3)-Si(H) (C_{59}Si) was observed. The L-configuration possessed the lowest symmetry and narrowest energy gap of all the possible configurations.

The radii and lengths of the SWCNTs had effects on the first absorptions of the doped SWCNTs. The first absorptions of (3,3)-Si(L) (C_{35}Si), (4,4)-Si(L) (C_{47}Si) and (5,5)-Si(L) (C_{59}Si) were gradually red-shifted. The analogous red-shift in the first absorptions of (3,3)-Si(L) (C_{35}Si), (3,3)-Si(L) (C_{47}Si) and (3,3)-Si(L) (C_{59}Si) appeared.

3.4. ^{13}C NMR Spectra

The chemical shifts of the carbon atoms connected with the silicon atom in the doped SWCNTs generally moved upfield, in comparison with those in the pristine SWCNTs (Table 3). The silicon atom owned an electron-donating character, and the carbon atoms nearby displayed the strong electronegativity. The electron density on these carbon atoms was elevated, and the shielding effect was strengthened.

The chemical shifts of the carbon atoms were relevant to the size of the SWCNTs as well. The chemical shifts of the same carbon atoms in (3,3) (C_{36}), (4,4) (C_{48}) and (5,5) (C_{60}) moved downfield successively, and those of the carbon atoms in (3,3)-Si(L) (C_{35}Si), (4,4)-Si(L) (C_{47}Si) and (5,5)-Si(L) (C_{59}Si) also progressively moved downfield. Besides, oscillation regularities in the chemical shifts of (3,3) (C_{36}), (3,3) (C_{48}) and (3,3) (C_{60}), as well as in those of (3,3)-Si(L) (C_{35}Si), (3,3)-Si(L) (C_{47}Si) and (3,3)-Si(L) (C_{59}Si) were observed.

3.5. Aromaticity

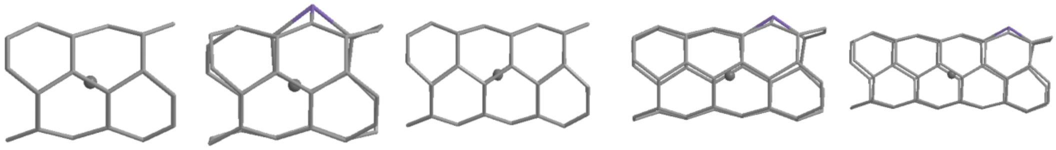
The NICS values higher than 5 indicated the anti-aromaticity of SWCNTs, whereas the NICS values lower than -5 showed the aromaticity [45-47]. The NICS values at the tube center of (3,3) (C_{36}), (3,3) (C_{48}) and (3,3) (C_{60}) were progressively decreased (Fig. 2). It could be predicted that the NICS values would be further decreased with the increase in the lengths of the SWCNTs. Thus, the aromaticity would be created if the lengths of the SWCNTs were enough. The NICS value

Table 2. The first absorption peaks in the UV Spectra of the SWCNTs calculated using INDO/CIS method

SWCNTs	(nm)	Doped SWCNTs	(nm)
(3,3) (C_{36})	747.0	(3,3)-Si(L) (C_{35}Si)	806.2
(3,3) (C_{48})	734.7	(3,3)-Si(L) (C_{47}Si)	880.9
(3,3) (C_{60})	937.5	(3,3)-Si(L) (C_{59}Si)	1056.2
(4,4) (C_{48})	977.8	(4,4)-Si(L) (C_{47}Si)	818.6
(5,5) (C_{60})	937.5	(5,5)-Si(L) (C_{59}Si)	973.9

Table 3. The chemical shifts of the carbon atoms in the SWCNTs at B3LYP/6-31G(d) level

SWCNTs	Chemical Shifts (ppm)	Doped SWCNTs	Chemical Shifts (ppm)
(3,3) (C_{36})	144.7	(3,3)-Si(L) (C_{35}Si)	122.3
(3,3) (C_{48})	138.4	(3,3)-Si(L) (C_{47}Si)	185.9
(3,3) (C_{60})	144.1	(3,3)-Si(L) (C_{59}Si)	119.4
(4,4) (C_{48})	150.5	(4,4)-Si(L) (C_{47}Si)	126.8
(5,5) (C_{60})	154.7	(5,5)-Si(L) (C_{59}Si)	147.1



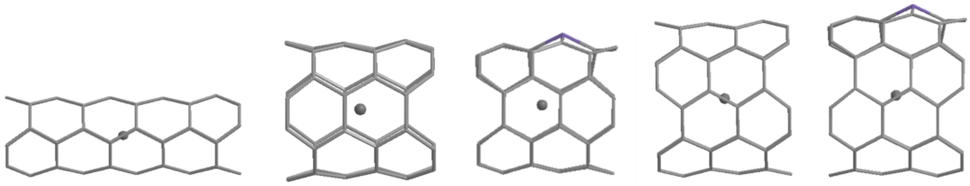
(3,3) (C_{36})
NICS = 6.3

(3,3)-Si(L) (C_{35}Si)
NICS = 1.8

(3,3) (C_{48})
NICS = 6.0

(3,3)-Si(L) (C_{47}Si)
NICS = 4.7

(3,3)-Si(H) (C_{47}Si)
NICS = -0.1



(3,3) (C_{60})
NICS = 2.9

(4,4) (C_{48})
NICS = 8.6

(4,4)-Si(L) (C_{47}Si)
NICS = 6.7

(5,5) (C_{60})
NICS = 7.7

(5,5)-Si(L) (C_{59}Si)
NICS = 6.0

Figure 2. The NICS values at the tube center of the SWCNTs at B3LYP/6-31G(d) level

of (4,4) (C_{48}) or (5,5) (C_{60}) was higher than that of (3,3) (C_{36}). Then the anti-aromaticity was intensified as the radius of the SWCNT increased.

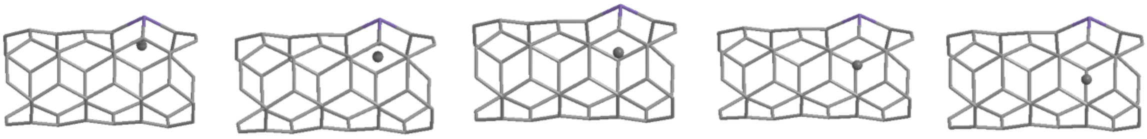
The NICS values of the doped SWCNTs compared with those of the pristine SWCNTs were decreased. The anti-aromaticity of the pristine SWCNTs was diminished upon the doping of the silicon atom. (3,3)-Si(H) (C_{47}Si) even displayed a negative NICS value. It could be concluded that the doping of the silicon atom was more favorable in producing the aromaticity than the increase in the lengths of the SWCNTs.

The change in the aromaticity of the system like benzoic acids [52] or fullerenes [31,32] could be characterized by the NICS scanning. Herein, the NICS scanning method was applied to (3,3)-Si(L) (C_{47}Si) in both the radial and axial directions. The helium atom was located in the cross section which contained the silicon atom. The initial position of the helium atom was near the silicon atom. The radial NICS scanning was performed by gradually moving the helium atom away from the silicon atom in the radial direction of (3,3)-Si(L) (C_{47}Si). The NICS values were observed to gradually decrease to the minimum then increase in the scanning process (Fig. 3). The silicon atom connected with the carbon atoms owned the electron-donating ability. The electron density on the silicon atom was decreased, and the shielding effect was reduced. Consequently, the other NICS values compared with the minimum moved downfield when the helium atom approached the silicon atom, whereas the NICS values moved upfield when the helium atom approached the opposite wall of (3,3)-Si(L) (C_{47}Si).

The axial NICS scanning was achieved by moving the helium atom from one end to the other along the axis of (3,3)-Si(L) (C_{47}Si). An oscillation dependence of the NICS values on the axial position of the helium atom was found (Fig. 4). This oscillation phenomenon was relevant to the heterogeneity of the hexagons in the aromaticity of the SWCNTs [51].

4. Conclusion

In summary, the doping of the silicon atom could be considered as an interference on the electronic structures of the SWCNTs. The weak interference would



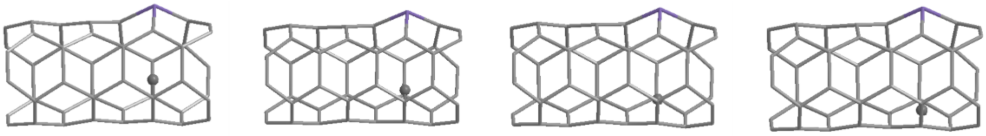
NICS = 8.4

NICS = 5.6

NICS = 3.6

NICS = 2.5

NICS = 1.8



NICS = 1.1

NICS = 0.2

NICS = 0.4

NICS = 2.3

Figure 3. Radial NICS scanning of (3,3)-Si(L) (C_{47}Si) at B3LYP/6-31G(d) level

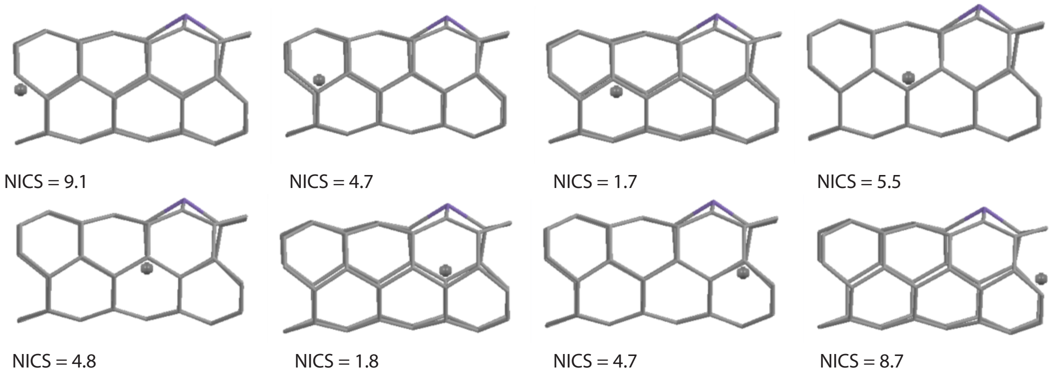


Figure 4. Axial NICS scanning of (3,3)-Si(L) ($C_{47}Si$) at B3LYP/6-31G(d) level

lead to the high thermodynamic stability of the SWCNT. The L-configurations of the doped SWCNTs were the most stable configurations of all. With the increase in the lengths of the doped SWCNTs, the energy gaps could be decreased and the reactivities were improved. The first UV absorptions for most of the doped SWCNTs compared with those of the pristine SWCNTs were red-shifted. The chemical shifts of the carbon atoms connected with the silicon atom in the doped SWCNTs relative to those of the corresponding carbon atoms in the pristine SWCNTs moved upfield. The aromaticity of the doped SWCNTs with respect to that of the pristine SWCNTs could be enhanced.

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