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Computational Investigations of Structural Stability, Electronic Structure, and Charge Density Analysis of Boron-Doped Single-Walled Carbon Nanotube

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Abstract

We perform the density functional theory (DFT) method to investigate the structural stability, the electronic structure, and the charge density distribution and transfer of the eight boron-doped (4, 0) single-walled carbon nanotube (B-doped SWCNT) systems. The eight B-doped (4, 0) SWCNT systems are distinguished by the number of B atoms substituting C atoms in a (4, 0) SWCNT structure. We find that all B-doped (4, 0) SWCNT structures are formed spontaneously marked by their negative formation energy. Also, all of these new systems have the stable structures. Then, surprisingly, we invent that the substitution doping B atoms retains the electronic properties of (4, 0) SWCNT. This is in contrast to other cases of impurities which alter the electronic properties of the doped structures. In addition, the distribution of charges between boron and carbon in the B-doped (4, 0) SWCNT structures indicates that there are electrostatic attractions between these two types of atoms. It shows that the presence of B atoms can be accepted by a defective (4, 0) SWCNT in order to establish a new integrated B-doped SWCNT structure.

Keywords

B-doped (4, 0) SWCNT; structural stability; electronic structure; charge density distribution; density functional theory (DFT)

Introduction

A single-walled carbon nanotube (SWCNT) is 1D materials formed by rolling up a graphene sheet into a cylinder shape considering a pair of indices, (*n, m*). These indices are usually used to describe the atomic structures of the SWCNT such as armchair, zigzag and chiral, by specifying the chiral vector of the SWCNT on the graphene net [1]. On the other hand, a SWCNT has a number of superior properties relate to the combination of the excellent mechanical, thermal, and electronic properties. Its density can be one-sixth of the density of stainless steel, and its stiffness can be 5x higher than that of stainless steel [2]. It also has a higher stability and a higher thermal conductivity (~3000 W/m/K) compared to diamond [3]. In addition, this nanotube can be a metallic or a semiconducting, so it can be said that the SWCNT has extraordinary electronic properties. Thus, the SWCNT is favorable to be applied in many fields and disciplines such as nanotechnology, electronics, construction, manufacturing, medicine and so on [4].

Nowadays, the SWCNT's applications are increasingly unlimited since its properties can be upgraded. Several ways to upgrade these properties are to provide defects and disorders in the SWCNT. The presence of both defects and disorders will modify all properties of the SWCNT including chemical reactivity, mechanical strength, optical absorption, electronic transport and so on. Although the aim of both a given defect and a given disorder are similar, but they are slightly different. Defects in the SWCNT mean the imperfections in the regular geometrical arrangement of the atoms in a SWCNT, while disorders can be described as a complicated form of defects since a disorder contains a wide distortion range from the perfect SWCNT, *e*.*g*. the substitutional dopants.

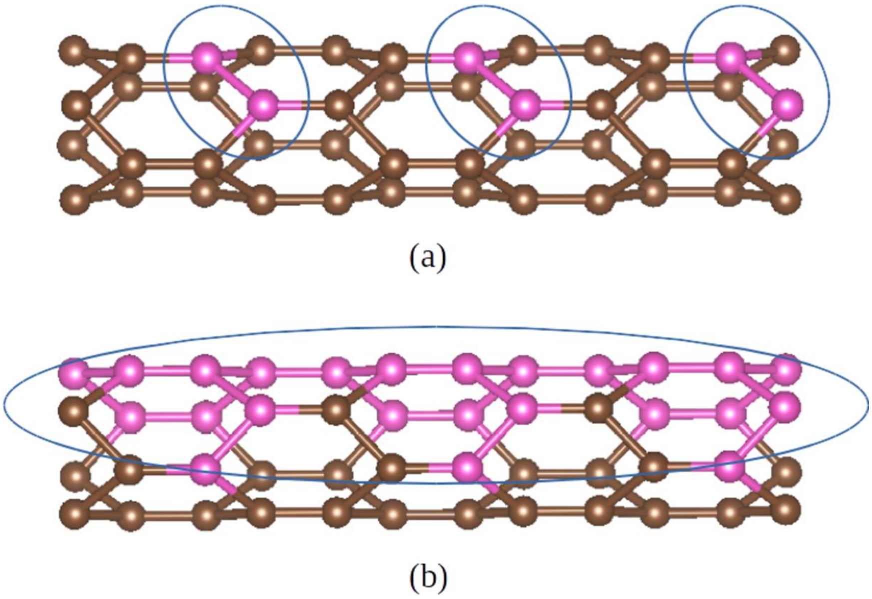
Actually, this kind of disorder have been investigated since decades ego, *i*.*e*. the substitutional doping of graphites using boron and nitrogen atoms and BN dimers have been investigated since the 1960s, and the similar techniques were applied to CNT and boron nitride nanotube (BNNT) in the 1995-1996 [5]. Then, doping of heteroatoms such as phosphorus [6], nitrogen [7], boron [8] and others, has been extensively explored.

Among all of these doping elements, we prefer to use boron to be a dopant in the SWCNT because of some considerations, that are: 1) The size of boron atom and carbon atoms are almost similar which means the stability of the structure can be maintained after doping because of a minimized lattice distortion [9]. 2) Boron doped SWCNT is highly potential to synthesis. There are several experimental works have been successfully synthesized this system. For example; Ding et al. suggested a synthesis technique with the combination of boron doping and fabrication of mesoporous carbon via application of sol-gel [10], Godfrey Keru et al. performed the chemical vapour deposition (CVD) floating catalyst method [11], Han et al. used the postsynthesis doping method by mixing CNTs with the boron-dopant at high temperature [12] and so on.

Based on the previous works, the enhanced properties of B-doped SWCNT resulted in the widely application such as; gas sensor [13], hydrogen storage [14], oxygen reduction reactions (15), transparent conducting film [16], lithium batteries [9], and supercapacitor [17]. However, there is an aspect that must be realized in many cases of a disorder such as the substitutional dopants (boron). The presence of boron atoms can be inconsequential or even beneficial depending on the application. For example: Fakhrabadi et al. claimed that 5% boron doping drastically reduces the thermal conductivity of CNTs more than 65% [18]. This is a disadvantage for applications requiring a high thermal conductivity. That is, not all of the findings match our expectations.

This undesirable thing (failure) can be minimized by doing the computational studies before going directly to the experimental works. It is a reason that prompted us to conduct a computational study of the basic properties of B-doped SWCNT before considering an experimental work and its applications, in view of the required cost of an experimental work is expensive.

In this work, we are developing the new idea of the B-doped SWCNT work. First, we prefer to use the small size of SWCNT (*d* <1 nm) such as (4, 0) SWCNT rather than the large size. We believe that there are unique things can be obtained from a small size SWCNT investigation compared to a large size SWCNT, whose properties are almost like graphene. In addition, the ultra-small diameter of SWCNT has been successfully synthesized by Thang et al. [19]. Therefore, this work is realistic for experimental work in the near future. Second, boron atoms as the dopants will substitute carbon atoms in the pristine SWCNT. We establish eight models of the new B-doped SWCNT structures in which boron atoms are designed to be closer to each other. It is based on a consideration that the energy to generate the second defect, the third defect and so on, after the first defect is formed, is lower than the energy required to create two separated single defects [20]. Third, a new hybrid material called carbon boron nanotube (CBNT) has generated from our work. As seen in Figure 1, we perform the isolated (4, 0) SWCNT which periodically repeated along its axis. As we put two B atoms to replace two C atoms in a unit cell of the (4, 0) SWCNT, this system and its pattern will be repeated when we develop a super cell containing infinite unit cells as shown in Figure 1(a). Consequently, as the number of B atoms increases to half the population of all atoms, the new hybrid called (4, 0) CBNT as shown in Figure 1(b), will be produced.


(a)

(b)

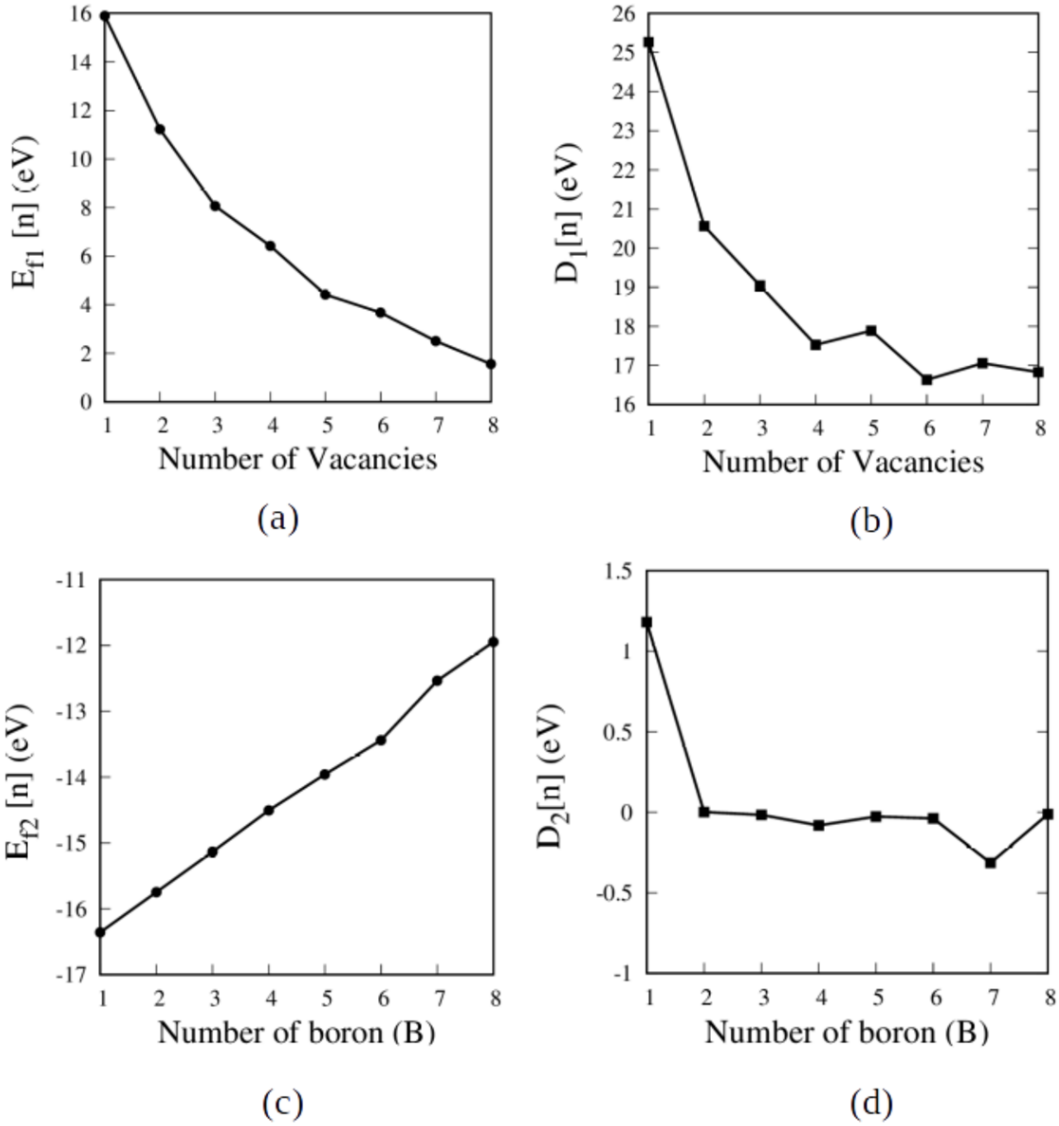
Figure 1: The (4, 0) SWCNT isolated systems are periodically repeated along the nanotube axis; a) two B atoms doped (4, 0) SWCNT, b) eight B atoms doped (4, 0) SWCNT. (Brown: carbon and pink: boron).

Hereinafter, the density functional study (DFT) is conducted to calculate the basic properties of B-doped (4, 0) SWCNT such as; the dissociation energy and the formation energy which relate to determine the structural stability, the electronic structures, and the charge density distribution using Bader's analysis. These calculations are essential to be carried out before proceeding with the next investigation.

Results and Discussion

Structural Stability

We specify the two conditions to describe the details of the substitutional doping processing. First, as the vacancies in the (4, 0) SWCNT are formed. Second, as the boron atoms are filled the vacant sites of the (4, 0) SWCNT. These are adopted as an illustration of B-doped SWCNT. However, both of these conditions may be occurring very rapidly in practice, and the interval of these two events has yet to be determined. It is caused since boron will charge the vacant positions as soon as the carbon was released in the experimental works. So, there shouldn't be an assumption that a vacant structure will disintegrate before a boron occupy that vacant site. By considering these thoughts, the four graphs are obtained as shown in Figure 2. Each graph will be described in detail as follows.



(a)

(b)

(c)

(d)

Figure 2: (a) The formation energy of the vacant (4, 0) SWCNT, (b) The dissociation energy of the vacant (4, 0) SWCNT, (c) The formation energy of the B-doped (4, 0) SWCNT systems, and (d) The dissociation energy of the B-doped (4, 0) SWCNT systems.

First, we represent the formation energy of each SWCNT related to the number of C atoms which removed from their origin position called vacancies. We need to define the formation energy of the (4, 0) SWCNT as the energy required or released while generating the configuration of these vacancies. We note that what we refer to as “formation energy”, is different from the free energy (Gibbs) of formation or the heat (enthalpy) of formation, which used in Physical Chemistry. The free energy and the enthalpy contain contributions of translational, rotational, and vibrational degrees of freedom. However, in our case, we work with energies provided by a DFT code, which are potential energies within the framework of the Born-Oppenheimer approximation. It briefly explains that we are allowed to fix the positions of the nucleus and determine the energy of the system as the sum of the kinetic energy of the electronic cloud and the energy of the Coulomb interactions between electrons and nucleus. Thus, the formation energy of these vacancy systems is shown in Figure 2(a).

Based on Figure 2(a), all vacancy systems cannot be spontaneously formed. It takes a lot of energy to build these configurations. The greatest energy required is to take one C atom from its origin position. This required energy will then decrease by increasing the number of C atoms removed. The concept is that it is easier to add defects to an already compromised system. Thus, forming a second vacancy requires less energy than forming the first vacancy, and so on. On the other hand, it is also reasonable that it takes more energy to create the first vacancy than to build the second vacancy, and so on, since it needs a lot of energy to break the three strong C-C bonds at the first vacancy compared to the second vacancy, which has only two C-C bonds (see Figure 5). This explanation is confirmed by the support of Figure 2(b).

Figure 2(b) shows the amount of energy needed to break down certain C-C bonds in order to create vacancies in which one C atom, two C atoms, three C atoms are removed from those systems until eight C atoms are removed. The data distribution in this graph has the same trend as in Figure 2(a). The more C-C bonds that were broken, the less energy needed to break the next C-C bonds. However, there is a slight fluctuation in energy between 5 and 8 vacancies. The energy required to break the C-C bonds on the 5th atom is 0.3 eV is greater than the energy needed to break the C-C bonds on the 4th atom. This also occurs for the 7th atom, which requires an energy of about 0.4 eV greater than the energy needed to break the C-C bonds in the 6th atom. Because the energy differences are not large, these fluctuations are acceptable, and they are likely to stagnate at a certain point. It could happen that the more atoms that have been released, the energy needed to release the next atoms will be saturated at the same rate.

Second, the formation energies of B-doped (4, 0) SWCNT refer to the number of B atoms in each structure are shown in Figure 2(c). All new structures can be formed spontaneously based on the negative signs in each their formation energy. The largest energy release to generate the first B-doped (4, 0) SWCNT system (B1). It's followed by B2, B3,... and B8 system, which ordered from the largest to the smallest of the released energy. Then, the most stable structure among the eight systems is also B1. It is also supported by the Figure 2(d) in which this system has the highest dissociation energy among the others.

Furthermore, Figure 2(d) has an interesting pattern of the dissociation energy. There is a positive sign of the dissociation energy of B1 system which means that this system will take some energy (1.18 eV) to break its B-C bonds. However, the other dissociation energies are slightly fluctuated around 0 eV. Almost of them have the negative dissociation energy. It means that they release some energy to break their bonds.

Electronic Structures

The pristine (4, 0) SWCNT is a metallic nanotube. As we substitute some of C atoms in its structure with B atoms, it keeps its metal properties. This result is different from the previous works of Qing Bo et al. [21] and Raad Chegel [22]. Qing Bo et al. used the (*n*, 0) nanotubes with *n* varying from 8 to 19. They declared that their results are consistent with the theory of Mele et al. that the changes of the electronic properties induced by low B substitution can be explained by a rigid-band shift model. They assumed that the Fermi level would be shifted downwards due to the missing π electrons from the boron atoms, while the valence-band structure would remain undisturbed [23]. Hereinafter, Raad Chegel performed two systems consisting of B-doped (20, 0) CNT and B-doped (21, 0) CNT. He stated that the direct B substitution creates a new band below the Fermi level and leads to invention of *p*-type semiconductor.

Meanwhile, this work employs a very small diameter nanotube, which is about 0.35 nm. There is almost no change in their band structures as we put different concentrations of B atoms in that structure as shown in Figure 3. Although their Fermi levels are slightly fluctuating with the amount of boron doping, in reality, this does not open up their band gaps. However, our results are reasonable as the presence of B atoms in the SWCNT makes the band gap of some type of SWCNT (semiconducting SWCNT) narrower than the band gap in its pristine structures [22]. Since the pristine (4, 0) SWCNT does not have a band gap, it makes sense if there is still no band gap after the substitution of boron atoms. This may be a failure if the objective of the work is to obtain semiconductor material for applications such as transistors, diodes, solar cells and others. However, this is advantageous for certain applications that wish to retain their metallic properties *e.g*. superconductors.

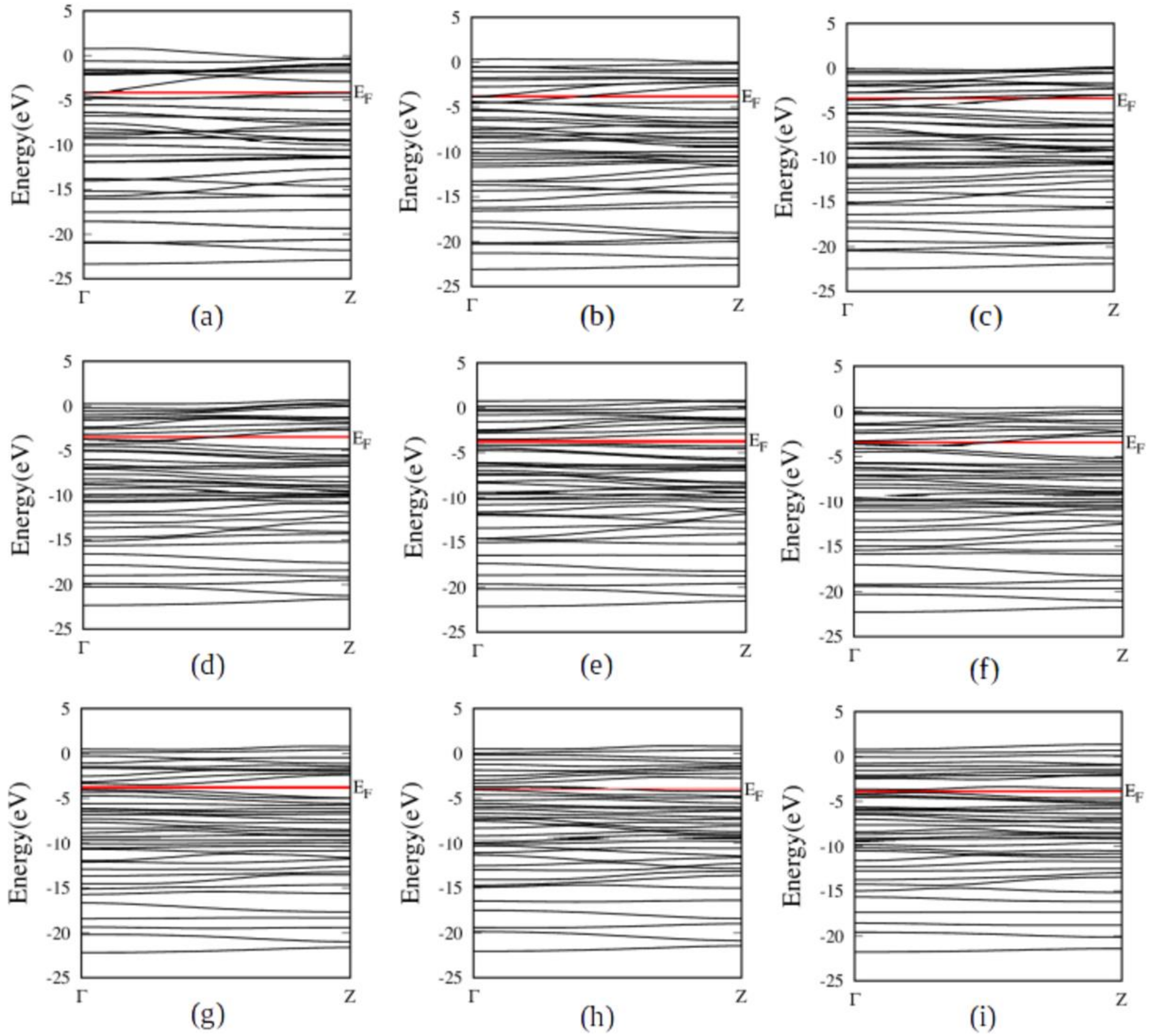


Figure 3: The band structures of: a) pristine (4, 0) CNT, b) B1, c) B2, d) B3, e) B4, f) B5, g) B6, h) B7 and (i) B8.

Charge Density Analysis

The properties of materials are frequently represented in terms of charge distribution or transfer between atoms and the presence of ionic charges on atoms or molecules [24]. We employed the Bader charge analysis method as we have declared in the computational section, to obtain a better perception for the charge distribution of B-doped SWCNT systems. It is emphasized that the calculation of this charge distribution is carried out after the adsorption process (B-C bonds already formed in the B-doped system). Thus, that charge distribution between C atoms and B atoms can be seen in Figure 4, Table 1 and Supporting Information File 1 in details.

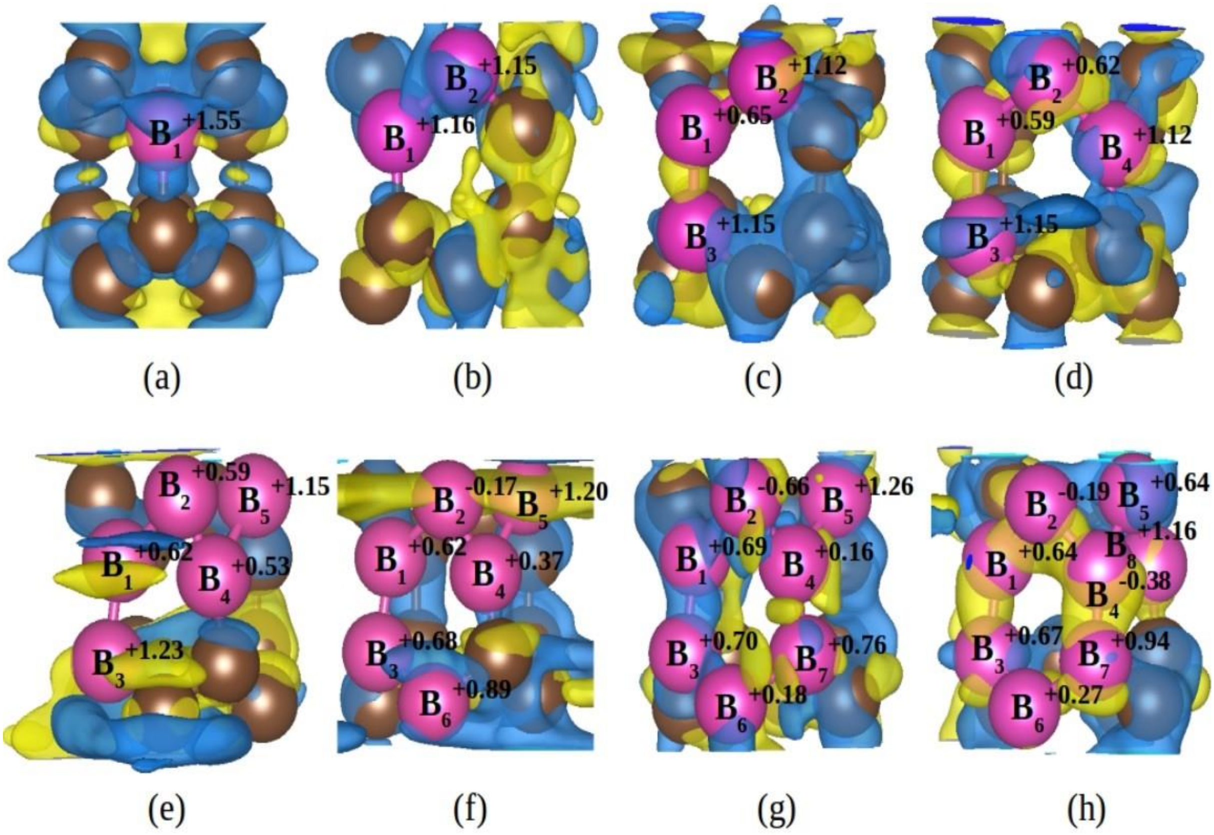


Figure 4: The 3D charge density distributions of B-doped (4, 0) SWCNT for each system: a) B1, (b) B2, c) B3, d) B4, e) B5, f) B6, g) B7, h) B8. (brown: C atoms, pink: B atoms, yellow: negative charge, blue: positive charge).

Furthermore, we will describe the charge distribution for some of the B-doped (4, 0) SWCNT systems in Figure 4. Not all systems are explained in detail, because all data in each system are already shown in the 3D charge distributions as displayed in Figure 4, Table 1 and Supporting Information File 1. We take three systems such as B1, B2, and B6 in order to show readers how to read their charge distribution. For examples: 1) The B1 system represents a structure in which a C atom is substituted by a B atom in a (4, 0) SWCNT structure as shown in Figure 4(a). In this case, the total charge of the regions around B_1 atom contained 1.45 electrons and C atom regions contained

61.51 electrons, giving a total of 62.96 electrons. It means that 1.55 electrons are transferred from that B_1 atom to the surrounding C atoms since B actually has 3 electrons in its valence. 2). The B2 system shows a structure in which two C atoms are substituted by two B atoms in a (4, 0) SWCNT structure as seen in Figure 4(b). The total charge of 61.95 electrons consisting 1.84 electrons is located in each region of B_1 and B_2 atoms. Meanwhile, there are 58.27 electrons to be around C atoms. So that, there are 1.16 electrons are transferred from both B_1 and B_2 atoms to the surrounding C atoms. 3) The B6 system indicates a structure in which six C atoms is replaced by six B atoms in a (4, 0) SWCNT structure as displayed in Figure 4(f). Approximately 0.62 electrons, 0.68 electrons, 0.37 electrons, 1.20 electrons and 0.89 electrons are transferred by the atoms of B_1, B_3, B_4, B_5 and B_6 respectively. Meanwhile, a B_2 atom in this system accepts 0.66 electrons from its surrounding atoms. Since B_2 is more likely to accepts electrons, so the charge of B_2 atom is marked as negative (-0.66).

On the basis of these data, it can be stated that almost all B atoms in the B-doped (4, 0) SWCNT structure act as a charge donor. In the meantime, most of C atoms act as a charge receptor. These charge distributions show that B atoms can be adsorbed by the defective SWCNT systems, then forming the new B-doped (4, 0) SWCNT systems, which can be called the (4, 0) CBNT hybrid materials. This statement is also supported by the transfer of charges between the defective (4, 0) SWCNT structures (vacancies) and B atoms as shown in Table 1.

Table 1: The partial charge of carbon and boron in each B-doped SWCNT structure and the charge transfer ob- served in each B-doped SWCNT system.

Partial Charges								
Systems	B1	B2	B3	B4	B5	B6	B7	B8
C atoms	-0.50	-0.49	-0.56	-0.56	-1.19	-1.22	-0.57	-0.57
	-0.44	-0.58	-0.02	-1.15	-0.61	-0.57	-0.06	-1.24
	-0.02	-0.03	-1.07	-0.53	-0.53	-0.05	-1.19	-0.62
	+0.03	-0.53	-0.03	-0.08	-0.05	-0.55	-0.01	-0.13
	+0.02	+0.02	-0.03	-0.01	-0.47	+0.01	-0.07	-0.63
	+0.03	+0.02	-0.01	0.00	-0.03	-0.03	-0.61	+0.04
	-0.02	+0.03	-0.03	+0.03	-0.09	-0.60	-0.04	-0.04
	-0.07	-0.02	+0.04	+0.01	-0.57	-0.02	-0.02	-0.50
	-0.02	-0.04	-0.05	-0.64	-0.01	-0.03	-0.51	
	0.00	-0.02	-0.58	+0.04	-0.01	-0.49		
	-0.02	-0.06	+0.01	-0.06	-0.52			
	-0.50	-0.01	-0.03	-0.49				
	-0.02	-0.07	-0.52					
	+0.03	+0.04						
	+0.02							
B atoms	+1.55	+1.16	+0.65	+0.59	+0.62	+0.62	+0.69	+0.64
		+1.16	+1.12	+0.62	+0.59	-0.17	-0.66	-0.19
			+1.15	+1.15	+1.23	+0.68	+0.70	+0.67
				+1.12	+0.53	+0.37	+0.16	-0.38

					+1.15	+1.20	+1.26	+0.64
						+0.89	+0.18	+0.27
							+0.76	+0.94
								+1.16
Charge Transfer (e/Å^3)	0.03	0.03	0.04	0.04	0.04	0.04	0.04	0.04

A charge transfer or an electron-donor-acceptor is a combination of two or more atoms or molecules in which a fraction of the electronic charge is transferred between that atomic or molecular entities. Although the amount of charge transferred between the two systems is small, 0.03 e/Å^3 - 0.04 e/Å^3, this amount may be considered sufficient to ensure that the electrostatic attraction gives the B-doped (4, 0) SWCNT systems a stabilizing force.

Conclusion

We have investigated the structural stabilities, the electronic structures, and the charge distributions of eight B-doped (4, 0) SWCNT systems using DFT method. Each B-doped (4, 0) SWCNT system can be formed spontaneously. On the other hands, all eight systems can be said to be stable as long as the required energy or the released energy during the formation process can be properly maintained. However, as with most existing cases, the most stable systems are still the least defective systems, such as B1. Then, all B-doped (4, 0) SWCNT systems retain their metallic properties. They don't have a band gap, so they might be a good superconductor. In addition, both the charge distribution between C atoms and B atoms, and the charge transfer between the defective (4, 0) SWCNT systems and B atoms, indicate that they have sufficient the electrostatic attraction to build a coherent structure.

Computational Details

We operated an isolated (4,0) SWCNT consisting of 16 carbon atoms in one unit cell. An integer pair (4, 0) corresponds to the chirality index (n, m) in which $n = 4$ and $m = 0$ which named by zigzag. The (4, 0) SWCNT has a stable structure with -17.62 eV of binding energy. Because its stability is quite high, substitutional doping the pristine (4, 0) SWCNT with boron atoms will make the hybrid structures can maintain their stability. Then, we put the concentration of boron in the pristine (4, 0) SWCNT up to 50 percent of all atoms in that pristine (4, 0) SWCNT. So, we get eight different systems based on the number of boron atoms in each structure.

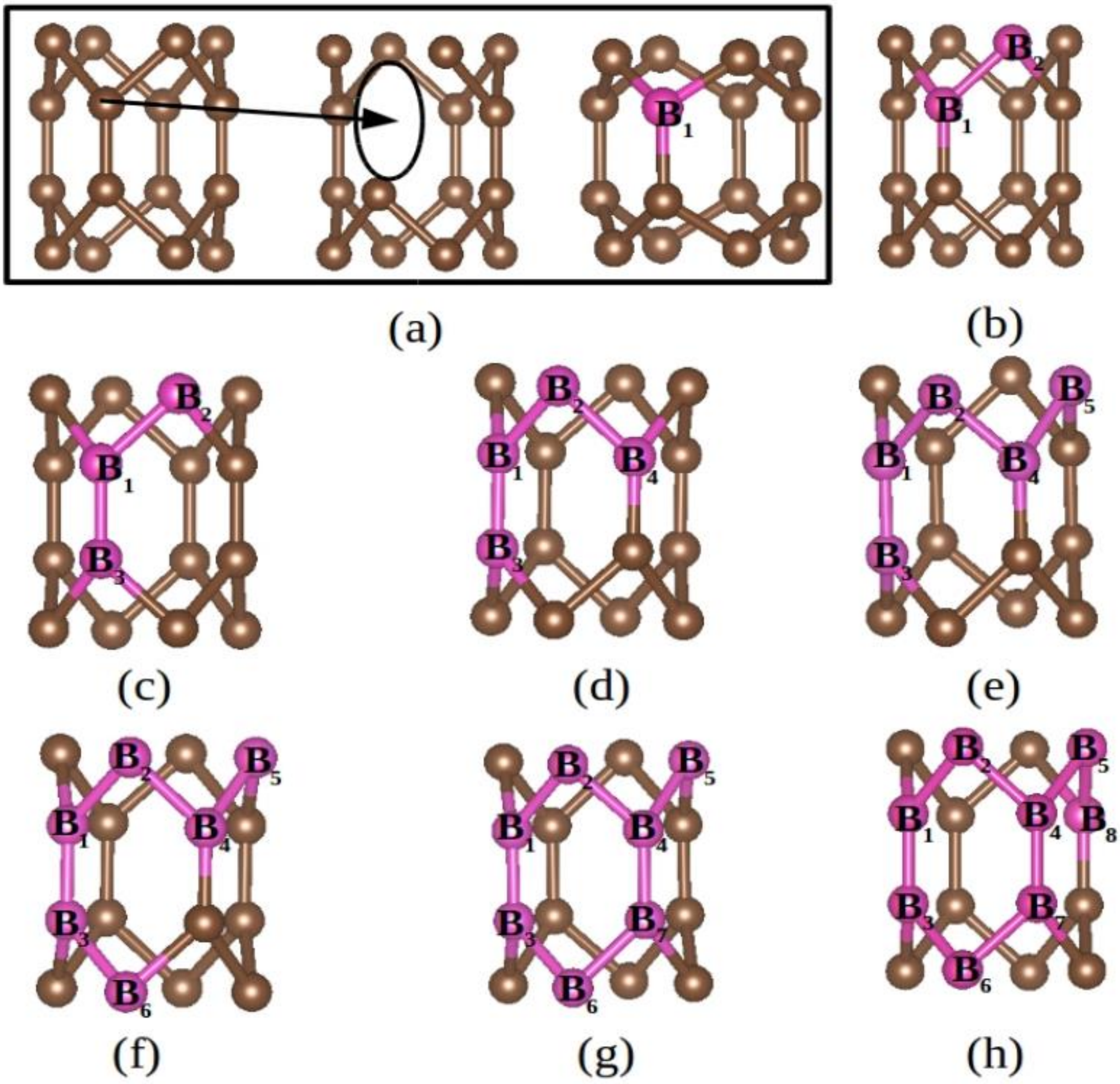


Figure 5: Eight systems of B-doped (4, 0) SWCNT. Each structure is labeled as: a) B1, b) B2, c) B3, d) B4, e) B5, f) B6, g) B7, and h) B8. (Note: brown: C atoms and pink: B atoms).

We established a B-doped (4, 0) SWCNT system by performing the three steps as illustrated in Figure 5a. First, we built an optimized pristine (4, 0) SWCNT structure. Second, we specified a vacancy in the pristine (4, 0) SWCNT by pulling out a carbon atom from its position. Last, we put a boron atom in this vacant site to substitute a carbon atom in that (4, 0) SWCNT. We remarked this system as B1. Then, the second and last steps were repeated in order to obtain B2, B3, B4,..., and B8 systems, in which their structures are shown, respectively, in Figure 5(b), Figure 5(c), Figure 5(d), and so on.

Afterward, the structural stability of these systems was determined by the calculations of their formation and dissociation energy. However, we have previously considered two conditions for specifying the structural stability of each system; a) As the vacancies had been generated. Here, we calculate the formation energy of the (4, 0) SWCNT with vacancies labeled as E_{F1} [*n*], and also their dissociation energy marked as D_1 [*n*]. b) At the time of the substitutional doping had been formed. We determine both the formation energy of the B-doped (4, 0) SWCNT system denoted by E_{F2} [*n*], and the dissociation energy of the B-doped (4, 0) SWCNT system pointed by D_2 [*n*]. Then, E_{F1} [*n*], E_{F2} [*n*], D_1 [*n*], and D_2 [*n*] are described using the following formula:

$$E_{F1}[n] = E_T[n] - E_F[n] - n\mu_C \tag{1}$$

$$E_{F2}[n] = \frac{E_{B-dopedSWCNT} - n_C\mu_C - n_B\mu_B}{N} \tag{2}$$

$$D_1[n] = D_2[n] = E_F[n-1] + E_f[1] - E_F[n] \tag{3}$$

where E_T [*n*] is the total energy of the reconstructed (4, 0) SWCNT with vacancies, E_p [*n*] is the total energy of the pristine (4, 0) SWCNT, n_C is the number of carbon atoms removed from the system and μ_C is the cohesive energy per atom of a single graphene sheet [25]. Then, $E_{B\text{-}doped\ SWCNT}$ is the total energy of the B-doped SWCNT systems, n_B is the number of boron atoms inserted in the vacant sites of the (4, 0) SWCNT, and μ_B is the cohesive energy per atom of a boron flat sheet [26]. In addition, it is necessary to emphasize the use of the [*n*] symbol. The [*n*] symbol means the number of C atoms is taken from the pristine (4, 0) SWCNT for E_{F1} [*n*] and D_1 [*n*]. However, the definition of

[*n*] changes to the number of B atoms is put into the vacant sites of the (4, 0) SWCNT for E_{F2} [*n*] and D_2 [*n*].

All of the required data for these calculations are conducted using the density functional method (DFT) within the VASP code [27, 28]. Not only for the calculation of ground state energy, but also for the determination of the band structures and the charge density distributions (Bader's analysis). Then, the Perdew-Burke-Ernzerhof (PBE) approximation is used as an exchange correlation energy with ultrasoft-pseudopotential [29, 30]. The energy cutoff and the number of k-points are set at 550 eV and 18 k-points along the reciprocal axis of the (4,0) SWCNT. These calculations are completed when the energy differences and the Hellmann Feynman forces are converged to 10^{-5} eV and -0.01 eV, respectively.

Supporting Information

Supporting Information File 1

Additional charge distribution data of all eight B-doped (4, 0) SWCNT systems.

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