Energetics and stability of hydrogen sulphide adsorption on defective carbon nanotube

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Abstract: We investigate a new design of the defective zigzag (10,0) carbon nanotube (CNT) as a hydrogen sulphide (H_2S) sensor using density functional theory (DFT). Herein, the defective zigzag (10,0) CNT obtained by removing one to five carbon atoms from the pristine zigzag (10,0) CNT to create simultaneously one to five of the single vacancies located around the nanotube axis. The formation energy and the dissociation energy inform us that all defective zigzag (10,0) CNT systems are stable. Then, the adsorption energy shows that these defective systems can adsorb the H_2S molecules. Furthermore, an unexpected finding has also been found in this study. The presence of the H_2S molecules on the defective (10,0) CNT arises the band gap of these systems.

Keywords: defective CNT; formation energy; dissociation energy; adsorption energy; H_2S sensor; density functional theory.

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1 Introduction

The properties of carbon nanotube (CNT) are influenced by its geometry such as chirality, nanotube diameter, length, and morphology (Oftadeh et al., 2013). For example, CNT can be a conductor or a semiconductor depending on its chirality (Rao et al., 2001). The properties of CNT can also be changed by giving the defects. Several types of defects that have been introduced are Stone-Wales, adatoms, and vacancies (Amorim et al., 2007; Ewels et al., 2003; Stone and Wales, 1986).

Vacancies are an interesting topic to be investigated. Vacancies are common and are generated after the CNT synthesis. The single-walled CNT (SWCNT) has a frequently spontaneously possibility of vacancies compared to the multi-walled (MWCNT). For example, the single vacancies may occur during annealing process, even they are observed to merge into wider void. On the other hand, knocking-on the CNT structures using high energy electron, ion, or neutron radiation can dislodge one or more C atoms. However, the energy to knock-on CNT must be considered precisely in order to gain synthetic control over materials design. For example, it requires 5–6 eV of energy to create a vacancy in the graphite. In addition, the di-vacancy created by two missing C atoms needs just 1 eV more energy than the mono-vacancy requirement, and almost 6 eV less than two separated mono-vacancy requirements (Collins, 2010). These conditions also apply to CNT with the different energy calculations.

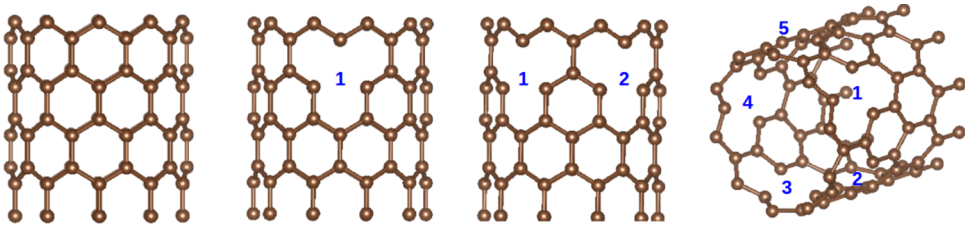
Hereinafter, the computational studies of the existence of vacancies in both graphene and CNT have been reported by Saito et al. (2007) and by Padilha et al. (2011). The authors apply vacancy models ranging from a single vacancy to an octovacancy in such a way that a large cavity in CNT is formed. The authors also state that the divacancy, the tetravacancy and the hexavacancy are the most stable in both a graphene sheet and a CNT (Padilha et al., 2011).

Vacancies in CNT can be used as binding sites for gaseous in the CNT-based sensors (Rocha et al., 2008; Yamashita et al., 2006). A quick response time and a high sensitivity of CNT to the gas molecules after adsorption, generate the change in electrical conductivity is particularly favourable for gas sensor applications (Collins et al., 2000). In addition, some literatures also state that CNT is a good sensor for many gases, such as O_2 (Collins et al., 2000), NH_3 (Feng et al., 2005), NO_2 (Li et al., 2003), SO_2 (Ciraci et al., 2004) and C_2H_2 (Yusfi et al., 2020).

Furthermore, CNT is not only applicable as sensors of those gases, but also CNT can perform as a valuable candidate for hydrogen sulphide (H_2S) sensors. It is very important to detect the presence of H_2S gas in various industries such as coal mining, oil and extraction gas and other industries. H_2S gas is known to be very harmful to humans because it is poisonous and highly flammable even in low concentrations. Current sensors use materials such as SnO2-CuO multilayered, Ag/Ag2S electrode, and heterostructured p-CuO (nanoparticle)/n-SnO2 (nanowire) devices (Shao et al., 2013; Zhang et al., 2013; Verma and Gupta, 2012). They work at high temperature, so that these sensors need high cost and high power consumption. Therefore, it is necessary to investigate a new material which shows a faster response, a higher sensitivity, a smaller size and a lower working temperature compared to the conventional gas sensor materials, such as CNT.

Actually, CNT as a H_2S gas sensor already simulated by Oftadeh et al. using density functional theory (DFT) (Oftadeh et al., 2013). Their work employed the pristine single-walled zigzag (5,0) and armchair (5,5) CNT. They selected (5,0) SWCNT containing 50 carbon atoms and 10 hydrogen atoms and the (5,5) SWCNT containing 100 carbon atoms and 20 hydrogen atoms. These indicate that they did not use the periodical systems, but they used clusters of zigzag (5,0) and armchair (5,5) CNT which terminated by hydrogen at both edges. Then, a H_2S molecule is placed in the vicinity of internal and external walls of these nanotubes. Their findings state that the thermodynamic quantities declare no simultaneous H_2S adsorption process while the natural bond orbital (NBO) analysis demonstrate a shift in the electronic structure of CNT which may be appropriate for fabricating the CNT sensors to provide a fast environment feedback.

Figure 1 The structure of the isolated single-walled (10,0) CNT: (a) pristine; (b) one atom vacancy employed/V_1; (c) two vacancies employed/V_2 and (d) five vacancies employed/V_5 (see online version for colours)



However, we still want the better results in this investigation. Our motivation is to make the CNT more sensitive as a sensor by designing defects in the pristine structure of CNT. This idea makes our work different from Oftadeh's work. The defective CNTs are designed by removing one until five C atoms from the pristine zigzag (10,0) CNT called vacancies. The vacant sites in the zigzag (10,0) CNT aim to make this material become

more reactive and sensitive to the presence of the H_2S gas compared to the pristine CNT structures. Thus, the H_2S gas can be easily adsorbed in these vacant sites. This work is also different from the work that had been investigated by Padilha et al. Here, we apply one to five of a single vacancy which are located around the nanotube axis as shown in Figure 1. So that, these vacancies generate a ring pattern that is different from their surroundings. In addition, all calculations including the formation energy, the dissociation energy, the adsorption energy and the band gap are performed by using the DFT.

2 Computational details

We performed a (m, n) CNT. A pair of integers m and n denotes the chirality of a nanotube. In this work, we used $m \neq n$, where $m = 10$ and $n = 0$. This structure is called the zigzag (10,0) CNT. Since its thickness is one C atom and it is isolated from the others, so this structure can be named an isolated single-walled zigzag (10.0) CNT. A zigzag (10,0) CNT was chosen because it has a moderate system consisted of 40 C atoms in one unit cell. However, we used a super cell consisted 80 C atoms to avoid a cluster of adjacent defects since we apply a periodic system. Furthermore, the curvature effect of a zigzag (10,0) is not too strong since its diameter is not too small (0.789 nm) with the C-C average bond length is 0.143 nm.

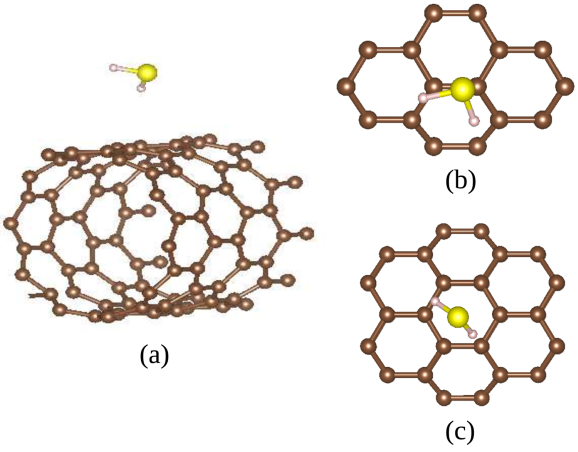
Based on its geometry, and related to our previous study, the zigzag (10,0) CNT is quite stable (Jonuarti et al., 2017). So that, if one or more C atoms are removed from the pristine zigzag (10,0) CNT, its structure will not immediately disintegrate and disperse compared to the smaller diameter nanotubes. The previous study also stated this nanotube is a semiconductor since it has a band gap around 0.908 eV (Jonuarti et al., 2017). A CNT semiconductor is interesting to investigate because we can directly see the impact of the defect on its electronic properties by looking at changes in its band gap before and after the defect.

Furthermore, we established a defect in the pristine zigzag (10.0) CNT after establishing a stable structure. The defective zigzag (10,0) CNT in this work is obtained by using a type of defect, such as atom vacancy, as shown in Figure 1. We employed five vacancies for this zigzag (10,0) CNT. It means one to five carbon atoms are removed from the pristine structure, thus generating five new structures with vacancy. These vacancies are remarked as V_1, V_2, V_3, V_4 and V_5 which correspond to the number of carbon atoms removed. Sites of two carbon atoms to five carbon atoms removed are circulated around the nanotube axis and are not directly neighbouring as displayed in Figure 1. Even though there are only V_1, V_2 and V_5 are shown in Figure 1, these structures already provide an overview of the V_3 and V_4 structures. Then, H_2S will be exposed to these systems.

An optimised H_2S structure has 0.13 nm of the average bond length (S-H) and 91.6° of the angle (H-S-H). Then, the H_2S molecules are located around the pristine zigzag (10,0) CNT and the defective zigzag (10,0) CNT. We set two sites of H_2S on the pristine zigzag (10,0) CNT as shown in Figure 2. Based on Figure 2, the bridge position is to place an H_2S molecule on top of the C-C bond, while the hollow position is to place an H_2S molecule on top of the hexagon. Furthermore, the positions of the H_2S molecules on top the defective zigzag (10,0) CNT are illustrated in Figure 3. We have five models of structures to represent the cases in which each H_2S is positioned at the top of the vacant

sites. The average distance between sulphur atom and the nearest of carbon atoms in both the bridge position and the hollow position is 0.4 nm after relaxing. The initial distance between sulphur and carbon atoms before relaxation was not considered. The optimum distance will be obtained after the relaxation process, which is indicated by the position of the sulphur atom changes to the most stable position and it becomes closer to the carbon atom if adsorption occurs.

Figure 2 (a) H_2S on top the pristine (10,0) CNT described into two positions; (b) bridge and (c) hollow (see online version for colours)



Brown: C, yellow: S and white: H.

All calculations are performed using DFT method within the VASP code (Kresse and Hafner, 1993; Kresse and Furthmüller, 1996). Then, the Perdew-Burke-Ernzerhof (PBE) approximation is used as an exchange correlation energy with ultrasoft- pseudopotential (Vanderbilt, 1985; Perdew and Wang, 1992). The energy cutoff and the number of k-points are set at 400 eV and 16 k-points along the reciprocal axis of (10,0) CNT. These calculations are completed when the energy differences and the Hellmann Feynman forces are converged to 10^{-6} eV and -10^{-2} eV, respectively.

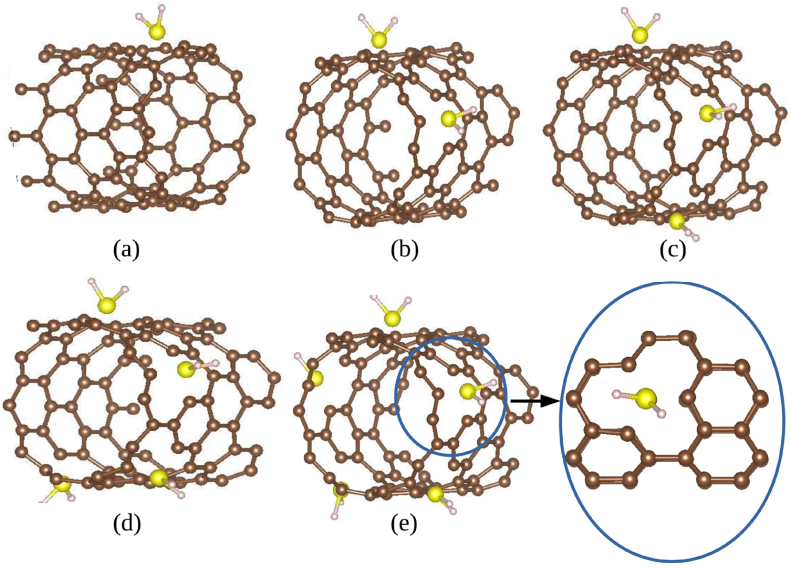
The calculated parameters such as the formation energy and the dissociation energy for the V_n vacancy (10,0) CNT are calculated using,

$$E_f[n] = E_T[n] - E_p[n] - n\mu_C \tag{1}$$

$$D[n] = E_f[n-1] + E_f[1] - E_f[n] \tag{2}$$

where $E_f[n]$is the formation energy, $E_T[n]$is the total energy of the reconstructured zigzag (10,0) CNT with a V_n defect, E_p is the total energy of the pristine zigzag (10,0) CNT, n is the number of carbon atoms removed from the system and μ_C is the cohesive energy per atom of a single graphene sheet (Zhuhua et al., 2009). Then, the dissociation energy described by the changing energy between initial and final states is remarked as $D[n]$, based on the assumption that a V_n defect breaks up into a single vacancy (Padilha et al., 2011). This dissociation energy belongs to the vacant systems. Equation (2) is to support equation (1), in which both of them prove the stability of the structures.

Figure 3 The positions of H_2S on top the defective (10,0) CNT; (a) V_1; (b) V_2; (c) V_3; (d) V_4 and (e) V_5 (see online version for colours)



Furthermore, the adsorption energy of H_2S on zigzag (10,0) CNT is described by the following formula:

$$E_{ads} = E_{CNT+H2S} - (E_{CNT} + E_{H2S}) \tag{3}$$

where $E_{(CNT+H2S)}$ is the total energy of the system, while E_{CNT} (adsorbent) and E_{H2S} (adsorbate) are the ground state total energy of the isolated zigzag (10,0) CNT and the isolated H_2S, respectively (Oftadeh et al., 2013). Since there are different kinds of systems are used, so that each component of equation (3) is further detailed as follows:

- *The pristine (10,0) CNT + H_2S*

The total energy of this system is the total energy of a system with complete number of C atoms in the pristine zigzag (10,0) CNT plus a molecule of H_2S. Then, E_{CNT} and E_{H2S} are the total energy of the isolated pristine zigzag (10,0) CNT (adsorbent) with complete number of C atoms and the isolated H_2S (adsorbate), respectively.

- *The (10,0) CNT with vacancies + H_2S*

The total energy of this system is the total energy of a system consisted of the (10,0) CNT with vacancies plus H_2S molecules. Meanwhile, E_{CNT} is adjusted to the total energy of the system, $E_{CNT+H2S}$. So that, E_{CNT} is the total energy of the isolated zigzag (10,0) CNT with vacancies (adsorbent). For example, a system described by two C atoms removed from the pristine structure of zigzag (10,0) CNT and two molecules of H_2S approached to the vacant sites, indicates that E_{CNT} + H_2S is the total energy of this system. Then, E_{CNT} is the total energy of the isolated zigzag (10,0) CNT in which two C atoms in this structure had removed, and $E$$H_2S$ is the total energy of two isolated H_2S (adsorbate).

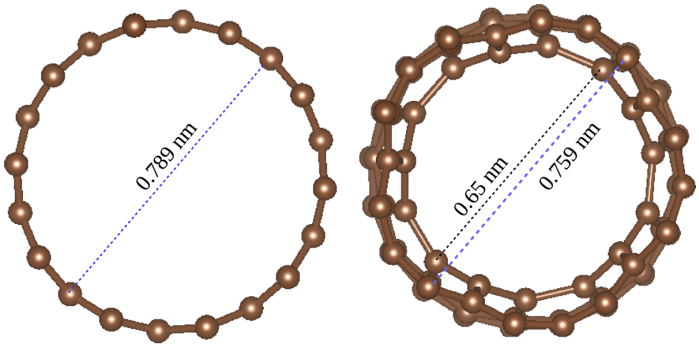
In addition, the isolated CNT and the isolated H_2S molecules are calculated at the same coordinates and scales of the lattice vectors as when the CNT + H_2S systems were constructed. Then, the DFT was performed to obtain the ground state energy of both the

isolated CNT and H_2S molecules using the same calculation order and functional as when the ground state energy of the CNT + H_2S system was measured.

3 Results and discussions

Figure 4 illustrates a difference between the pristine zigzag (10,0) CNT and the vacancy zigzag (10,0) CNT i.e., V_5 structure after relaxation. Figure 4(a) shows the diameter of the pristine zigzag (10,0) CNT is 0.789 nm in perfect cylinder shape. However, the V_5 zigzag (10,0) CNT has an irregular diameter. The C-C bonds around the vacant sites extend and retract in such a way as that will make the diameter around the vacant sites different from the other sections. So that, the inside diameter the V_5 zigzag (10,0) CNT is 0.65 nm while the outer diameter of this structure is 0.759 nm as pictured in Figure 4(b). However, All systems are stable related to their formation energy and their dissociation energy as shown in Figure 5(a) and (b).

Figure 4 The structures of: (a) the pristine (10,0) CNT and (b) the *V*5 vacancy (10,0) CNT (see online version for colours)

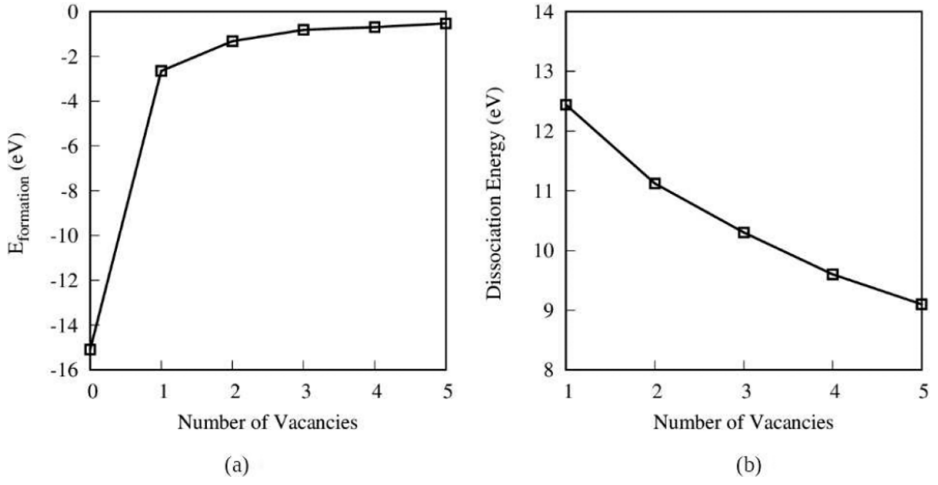


The formation energy vs. number of vacancies as shown in Figure 5(a) related to equation (1). There are five structures with vacancies denoted by V_1, V_2, V_3, V_4, and V_5 related to n = 1, 2, ..., 5 (number of vacancies). The V_1 means that one C atom is removed from the pristine zigzag (10,0) CNT structure, while the V_2 means that two C atoms are removed from that structure and so on. Then, the $E_f[1]$ denotes the formation energy for V_1 and so on. Furthermore, Figure 5(a) also shows the $E_f[0]$, which means n = 0 (there is no carbon atoms have been removed from the zigzag (10,0) CNT structure). So that $E_f[0]$ is the formation energy of the pristine zigzag (10,0) CNT. However, the presence of $E_f[0]$ in Figure 5(a) is only to show that the pristine structure has absolutely the greatest formation energy compared to the defective structures. Therefore, the main discussion is on the formation energy review of the defective zigzag (10,0) CNT structures.

The formation energy represents the energy required or released for generating that new configuration of molecules/systems within the reference set. Based on Figure 5(a), it takes more energy to reconstruct the V_1 structure than it takes to reconstruct the V_2 structure, and so on. The greater the energy required or released to build a structure, the more stable the structure would be. The order of the systems having the formation energy

from the largest to the smallest is V_1, V_2, V_3, V_4, and V_5, respectively (Figure 5(a)). Thus, it also means that V_1 is the most stable structure among the five structures with vacancies and then followed by V_2, V_3, V_4, and V_5 which respectively ordered from the greater stability to the least stability. Furthermore, a negative sign indicates that these systems have formed spontaneously.

Figure 5 (a) the formation energy as a function of the number of vacancies, and (b) the dissociation energy as a function of the number vacancies. (0: pristine, 1: V_1, 2: V_2, 3: V_3, 4: V_4, and 5: V_5)



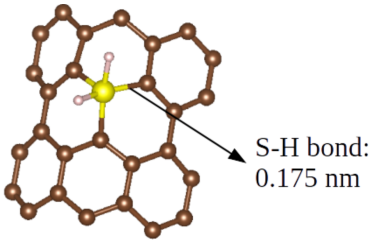
The stability of these structures are also described by Figure 5(b) which shows the relationship between the dissociation energy and the number of vacancies. The dissociation energy means the energy needed to break every chemical bond in a molecule and completely separate all its atoms. The greater the dissociation energy of a system, the more difficult to damage every chemical bond in a system, which means this system is stable. These dissociation energies in Figure 5(b) indicate that it is more difficult to break the C-C bond at V_1 than to break the C-C bond in V_2 and so on. This might be caused by that is easier to make the second vacancy after the first vacancy has formed. Therefore, the data in Figure 5(b) strongly support the data in Figure 5(a), which indicate that the V_1 structure energetically is the most favourable among the five structures with vacancies.

In addition, the dissociation energy corresponds to the bond energy. Since it takes energy to break a bond, bond energy are always positive (the negative sign simply means the amount of energy released when a bond is formed). As shown in Figure 5(b), we find almost 11 eV of an average energy dissociation value of C-C bonds. This value is reasonable since a vacancy in a zigzag (10,0) CNT breaks three short strong C-C bonds. It will increase the required energy to break three C-C bonds around the vacant sites. If the pristine zigzag (10,0) CNTs have a bond energy (bond dissociation enthalpies) of around 5 eV (Zeinalipour-Yazdi et al., 2019). Then, it is rational that the amount of the required energy to generate the defective zigzag (10,0) CNT is approximately twice or three times the amount of the bond energy (bond dissociation enthalpies) of the pristine zigzag (10,0) CNT.

Move on to other data, the interaction between the pristine zigzag (10.0) CNT with H_2S and the interaction of the V_1, V_2, V_3, V_4 and V_5 structures with H_2S molecules display

the signs of the adsorption formations. The H_2S locations were found to reach CNT after relaxation. The average bond length of S atom and the nearest C atom is 0.179 nm in which H_2S is on bridge or on hollow of the pristine zigzag (10.0) CNT. However, it is 0.175 nm in which H_2S is on an empty C position at zigzag (10.0) CNT as illustrated in Figure 6. Then, the average angle of the C-S-C is approximately 110°.

Figure 6 H_2S on an empty C site at (10,0) CNT (see online version for colours)



Then, the calculated energies of the H_2S molecules and the zigzag (10,0) CNT systems can be seen in Table 1. The total energy of these systems decrease as the number of empty C atoms increases and the number of the adsorbed H_2S molecules increases. However, this tendency does not apply to the adsorption energy. The CNT + H_2S systems in which H_2S on both hollow and bridge of the pristine zigzag (10,0) CNT and the CNT + H_2S systems in which H_2S on the vacant sites of the zigzag (10,0) CNT such as V_1, V_2 and V_3, have a negative adsorption energy. It means that the adsorption takes place spontaneously for these structures. On the other hand, there are slightly positive adsorption energies for V_4 and V_5 of the defective CNT + H_2S system. A slightly positive adsorption value means a little repulsion occurred between the interacting CNT and H_2S. The slightly positive adsorption energy is also possible to create bonds between carbon and sulphur, but these bonds will not stable.

Table 1 The total energy (E_{total}), the adsorption energy (E_{ads}), and the band gap (E_{gap}) of H_2S on (10,0) CNT system

System	E_{total} (eV)	E_{ads} (eV)	E_{gap} (eV)
H_2S on Pristine CNT			
Hollow	–738.59	–0.21	0.47
Bridge	–739	–0.24	0.93
H_2S on Defective CNT			
V_1	–724.04	–0.07	0.47
V_2	–720.69	–0.29	0.19
V_3	–717.16	–0.22	0.28
V_4	–713.66	0.04	0.28
V_5	–710.29	0.09	0.19

Hereinafter, the presence of the H_2S molecules on the structures of zigzag (10,0) CNT also affects the band gap of these structures. An H_2S molecule located on the bridge of the pristine structure (10,0) CNT reduces a value of its band gap to 0.74 eV. Whereas, an H_2S molecule located on the midpoint of the hexagon of the pristine zigzag (10,0) CNT,

actually increases the band gap energy to 0.93 eV. In addition, the systems of vacancies do not have a band gap, but after these systems adsorb the H_2S molecules, their band gap arises and appears to be a smaller value than the band gap value of the pristine zigzag (10.0) CNT.

4 Conclusions

We have calculated the formation energy and the dissociation energy associated with one to five of a single vacancy in the zigzag (10,0) CNT structure. We have shown that all vacant zigzag (10,0) CNTs such as the V_1, V_2, V_3, V_4 and V_5 structures are stable. Then, the H_2S molecules can be approached into these systems. The calculated adsorption energy indicates that the H_2S molecules are adsorbed spontaneously on the vacant sites of the zigzag (10,0) CNT structures, especially for the V_1, V_2 and V_3 system. Based on these results, the defective (10,0) CNT can be considered as an H_2S sensor.

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