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# Investigation of interaction hydrogen sulfide with (5,0) and (5,5) single-wall carbon nanotubes by density functional theory method

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**Abstract**

Herein, the interaction of hydrogen sulfide with inside and outside single-wall carbon nanotube of (5,0) and (5,5) is investigated using density functional theory at B3LYP/6-31G* level of theory in the gaseous phase by Gaussian 09. The adsorption energies, thermodynamic properties, highest occupied molecular orbital, lowest unoccupied molecular orbital, energy gaps, and partial charges of the interacting atoms are also studied during two kinds of rotation of hydrogen sulfide ($H_2S$) molecules as vertical and horizontal to the main axes of the nanotube. For these systems, the binding energy of $H_2S$-single-wall carbon nanotubes is low and the process is thermodynamically near-simultaneous.

**Keywords:** Hydrogen sulfide ($H_2S$), Single-wall carbon nanotube (SWCNT), Adsorption energy, Density functional theory (DFT)



## Background

The discovery of carbon nanotubes (CNTs) has caused considerable interest in many different scientific areas to investigate their physical and mechanical properties toward the development of potential technological applications. It has been demonstrated that theoretical methods and experimental procedures remarkably improve nanotube properties such as stiffness and strength [1]. Carbon nanotubes also have exceptionally high mechanical [2-4], electrical [5-8], and thermal conductivities [9-11] as well as high aspect ratio (length/diameter) and low density [12].

Single-walled carbon nanotube (SWCNT) properties are highly structure-/size-dependent and are influenced by atomic arrangement (chirality), nanotube diameter and length, and morphology or nanostructure. Depending on chirality, carbon nanotubes can either be conducting or semiconducting [13]. Wei et al. [14] demonstrated that multi-walled carbon nanotubes have extraordinarily high-current carrying capacity, sustaining current densities greater than 109 A/cm$^2$. These novel electrical properties have generated substantial interest in utilizing carbon nanotubes in nanoelectronics [15].

Sensing gas molecules is crucial for many process control technologies, and advances in chemical and physical sensors continue to get improved sensitivity, lower power consumption, and faster response. There is a strong demand for improved sensitivity, selectivity, stability, and low-power consumption beyond what is offered by commercially available sensors. In order to satisfy this demand, nanotechnologies are employed, providing new materials, devices, and systems with structures and components that can exhibit novel and significantly improved physical and chemical properties because of their nanoscale size [16]. The operation at the room temperature with sensitivity as high as $10^3$, besides their small size, is the main advantage of semiconducting-SWCNT sensors. The fast response of a nanotube sensor can be attributed to the full exposure of the nanotube surface area to chemical environments [17].

Seo et al. [18] reported the density-functional calculations of $NO_2$ adsorption on SWCNT. They found that $NO_2$ adsorption is both energetic- and kinetics-limited and strongly electronic structure and strain dependent. The $NO_2$ adsorption on metallic nanotubes was energetically more favorable than that on semiconducting nanotubes and, furthermore, the adsorption became less stable with

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increasing diameters of nanotubes. The diameter dependence of the adsorption energetics and kinetics in the chiral nanotubes are other important parameters in the adsorption process.

The effect of the shape and defect edge of SWCNT on the adsorption of $O_2$ and $N_2$ gases on the graphite has been studied theoretically by means of density functional theory coupled with cluster models [19,20]. The calculated adsorption energy 0.26 and 1.04 kcal/mol for $O_2$ and $N_2$, respectively, physisorbed on the clean basal surface, is in good agreement with the experimental value, suggesting that the one-layer simple cluster model is an effective way to investigate the adsorption of molecular gases on the graphite surface.

The doping effects of B and N on atomic and molecular adsorption of hydrogen in SWCNTs were investigated through density functional theory (DFT) calculations [21]. The results show that the B doping increases the hydrogen atomic adsorption energies both in zigzag and armchair nanotubes and a coordination-like B-H bond forms. The N doping decreases the hydrogen atomic adsorption energies.

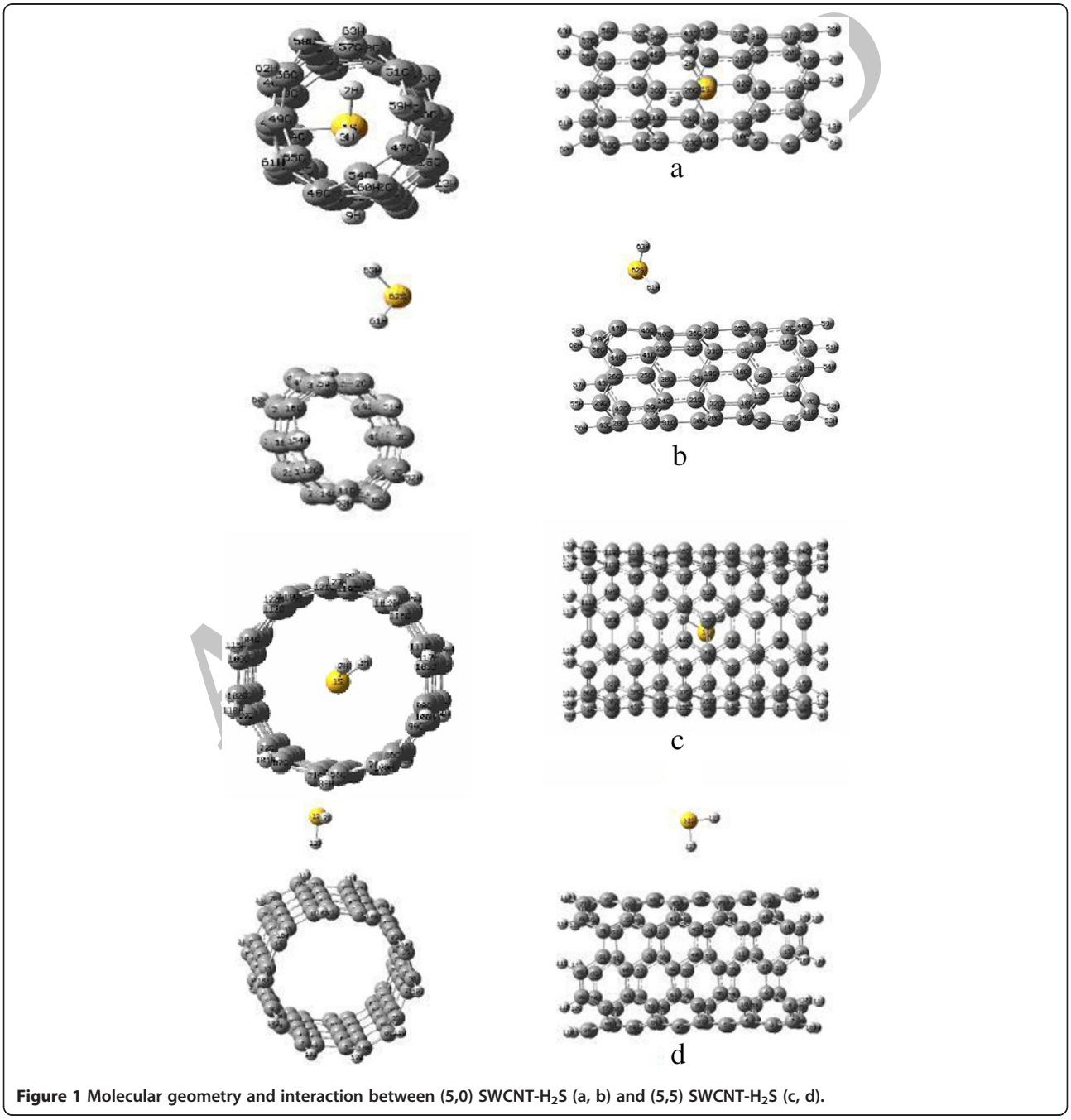


**Figure 1** Molecular geometry and interaction between (5,0) SWCNT-$H_2S$ (a, b) and (5,5) SWCNT-$H_2S$ (c, d).

**Table 1 Thermodynamic parameters**

| Optimized systems | ZPE | $\Delta U^0_{tot}$ | $\Delta H^0_{tot}$ | $\Delta G^0_{tot}$ |
|---|---|---|---|---|
| Internal of (5,0)-$H_2S$ | 335.0850 | 376.6882 | 333.7045 | 347.0703 |
| External of (5,0)-$H_2S$ | −1.0040 | 0.1883 | −0.3765 | 4.8947 |
| Internal of (5,5)-$H_2S$ | 32.8810 | 33.5712 | 32.9437 | 41.7915 |
| External of (5,5)-$H_2S$ | −0.3765 | 0.8158 | 0.3138 | 4.5180 |

Thermodynamic parameters including total zero-point energy, ZPE, total internal energy, $\Delta U^0_{tot}$, total enthalpy, $\Delta H^0_{tot}$, total Gibbs free energy, $\Delta G^0_{tot}$, (in kcal/mol) in the adsorption process of $H_2S$ molecule on the internal and external walls of (5,0) and (5,5) nanotubes calculated by B3LYP/6-31G*.

Humidity-assisted desorption of $SO_2$ and $NO_2$ has been experimentally investigated on carbon nanotubes [22]. The results showed that the resisted desorption of $SO_2$ on carbon nanotubes in dichloroethane solution increases at high humidity level (92%) and no change was observed in low humidity level, while there was also no change in desorption of $NO_2$ in the different levels of humidity.

There are many literatures about the carbon nanotube sensors as a detector for many much gases; for example, $O_2$ [23], $NH_3$ [17,24], $NO_2$ [25,26], and $SO_2$ [27]; and the change in electrical conductivity occurs after adsorption of molecules. These sensors have fast response time and high sensitivity to special gas molecules which is very favorable for certain applications [23].

There has been only few gas nanosensors developed for hydrogen sulfide ($H_2S$) detection including a catalytic chemiluminescence sensor made of R-$Fe_2O_3$ nanotubes [28], suppressed electron hopping occurred in gold nanoparticles [29], and networks made of hybrid polyaniline nanowires and gold nanoparticles [30]. There is little attention to the SWCNTs for this purpose because there is no chemical interaction with $H_2S$ or other gases that may interfere [31].

In the previous work, the effective parameters of (5,0) and (5,5) SWCNTs during the interaction with $CO_2$ as sensors were determined [32]. The interaction of $CO_2$ molecules and its rotation around tube axles vertically and parallel to internal and external walls of the nanotubes were studied using Gaussian 03 coding by density functional theory (DFT) at the B3LYP/6-311G level of theory. The carbon dioxide molecule was predicted to bind only weakly to nanotubes, and the tube-molecule interactions can be identified as physisorption. $CO_2$ adsorption is stronger on the external walls than on internal walls, and adsorption on the external wall of (5,0) is stronger than on the external wall of (5,5); the adsorption energies are exothermic. In the present study, the interaction of hydrogen sulfide with the inside and outside of (5,0) and (5,5) SWCNT is investigated.

## Method

### Computational method

Single-wall zigzag (5,0) and armchair (5,5) carbon nanotubes are considered. The diameters of the nanotubes are 4 and 6.85 Å, the lengths of the nanotubes are 8.5 and 9.8 Å, respectively, and the average bond length is 1.42 Å. The (5,0) SWCNT containing 50 carbon atoms and 10 hydrogen atoms and the (5,5) SWCNT containing 100 carbon atoms and 20 hydrogen atoms were selected for this purpose. Hydrogen sulfide in the vicinity of internal and external walls of the nanotubes is placed, and these structures are optimized by Gaussian 09 software [33].

DFT is used to study the structural and electric properties of the tube-molecule systems during adsorption of $H_2S$ molecule on the SWCNTs. In these cases the calculations are carried out with the B3LYP/6-31G* level of theory [34]. The geometry of all molecules under investigation is determined by optimizing all geometrical variables without any symmetry constraints. All optimization processes were carried out by supercomputer up to 32 processors via 20GB shared memory. The harmonic frequencies are computed from analytical derivatives for all species in order to define the minimum energy structures. Figure 1 shows the optimal structures.

The calculated parameters are the energy interaction of $H_2S$ with inside and outside wall of SWCNT, $E_{ads}$, through the following formula:

$$E\leftarrow\text{ads} = E_{\text{nanotube}-H2S} - (E_{\text{nanotube}} + E_{H2S}) \quad (1)$$

where $E_{\text{nanotube-H2S}}$ is the total energy of the optimized nanotube-$H_2S$ system, $E_{\text{nanotube}}$ is the total energy of the optimized nanotube and $E_{\text{H2S}}$ is the total energy of the isolated $H_2S$ molecule. By this explanation, $E$ads < 0

**Table 2 Effect of both adsorption of $H_2S$ molecule on the optical parameters of the systems**

| Optimized systems | $E_{ads}$ | BSSE | $E^{BSSE}_{ads}$ | HOMO | LUMO | $E_{gap}$ | Dipole moment (μ) |
|---|---|---|---|---|---|---|---|
| Internal of (5,0)-$H_2S$ | 0.5336 | 0.0100 | 0.5436 | −0.1667 | −0.1034 | 1.7218 | 0.8725 |
| External of (5,0)-$H_2S$ | −0.0027 | 0.0000 | −0.0027 | −0.1781 | −0.1149 | 1.7212 | 1.7648 |
| Internal of (5,5)-$H_2S$ | 0.0502 | −0.0060 | 0.0442 | −0.1596 | −0.0965 | 1.7109 | 0.4002 |
| External of (5,5)-$H_2S$ | −0.0024 | −0.0012 | −0.0036 | −0.1610 | −0.0985 | 1.6997 | 1.8597 |

The parameters, adsorption energy ($E_{ads}$), BSSE, $E^{BSSE}_{ads}$(in Hartree), HOMO, LUMO, gap energy (in eV), dipole moment, $\mu$, (in Debye), in the adsorption process of $H_2S$ molecule on the internal and external walls of (5,0) and (5,5) nanotubes, are calculated by B3LYP/6-31G*. BSSE, basis set superposition errors; HOMO, highest occupied molecular orbital; LUMO, lowest unoccupied molecular orbital.

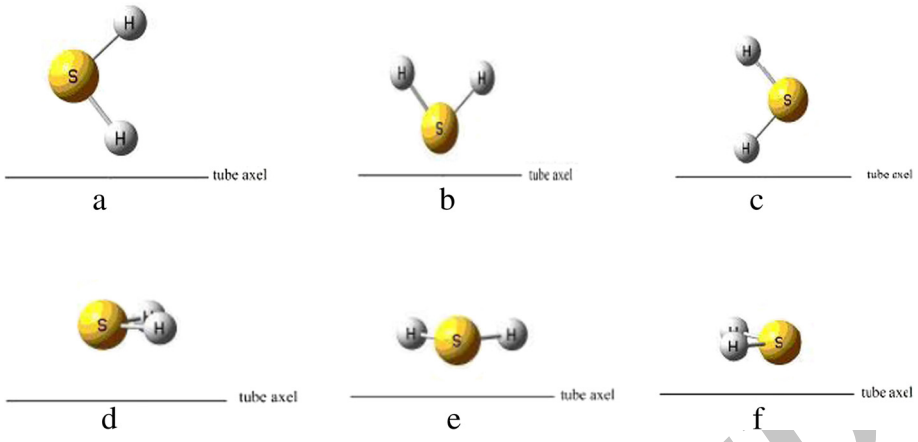


**Figure 2 Vertical and horizontal rotations around the tube axle.** Vertical (**a,b,c**) and horizontal (**d,e,f**) rotations around the tube axle at 0° (**a,d**), 90° (**b,e**) and 180° (**c,f**) angles.

corresponds to exothermic adsorption, which leads to a stable structure.

$$\Delta G^{0}{}_{tot} = \Delta G^{0}(H_2S - SWCNT) - \left[\Delta G^{0}(SWCNT) + \Delta G^{0}(H_2S)\right] \quad (2)$$

Total zero point energy, total internal energy, and total enthalpy are calculated to the same formula.

## Results and discussion

### Thermodynamic parameters

The results of the Gaussian output files, after tedious efforts for structure optimization with high-time-consuming thermodynamic parameters related to the electronic structure of (5,0) and (5,5) nanotubes in the presence of $H_2S$ molecule, in the vicinity of internal and external walls have been listed in Table 1. Total Gibbs free energy of $H_2S$-SWCNT system was calculated for inside and outside of (5,0) are 347.0703, 4.8947, and of (5,5) are 41.7915 and 4.5180 kcal/mol, respectively. Calculated Gibbs free energy shows that $H_2S$ adsorption process is not thermodynamically favorable. The lowest total zero-point energy, internal energy, and enthalpy relate to the process of $H_2S$ adsorption on the external wall of (5,0) nanotubes. The lowest Gibbs free energy is achieved during the interaction of $H_2S$ on the external wall of (5,5) nanotubes. Despite low and positive values of the Gibbs free energies of $H_2S$ adsorption on the external wall of (5,0) and (5,5) nanotubes, the adsorption energies are negative. It confirms no interaction between $H_2S$ gas and nanotube [15]. For obtaining more information, the optical properties under rotation of $H_2S$ molecule and natural bond orbital (NBO) analysis of $H_2S$ fluid-nanotube systems are studied.

### Optical parameters

The effect of both adsorption of $H_2S$ molecule on the optical parameters of the systems has been listed and compared in Table 2. The results show that the adsorption on the external is more effective than the

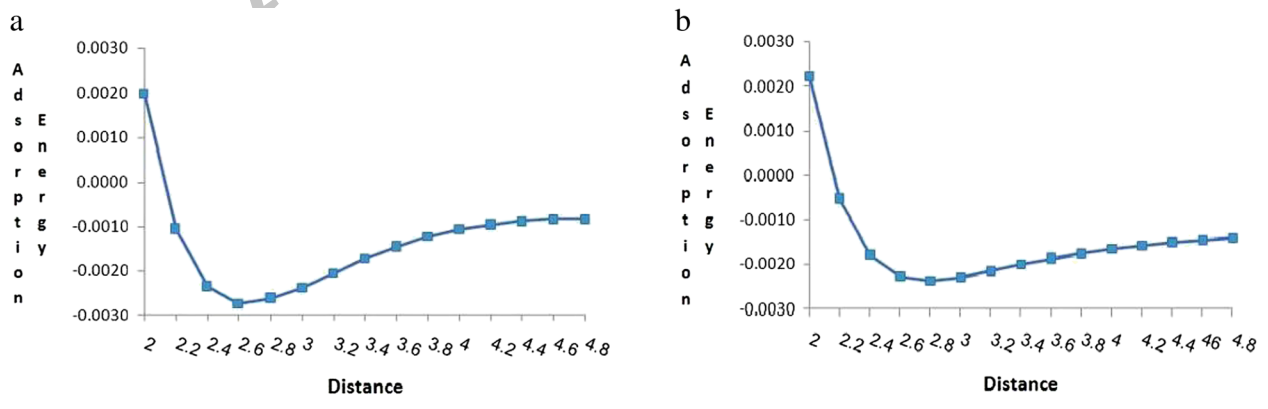


**Figure 3 Effect of $H_2S$ molecule distance on the adsorption energy.** The effect of $H_2S$ molecule distance on the adsorption energy from (5,0) SWCNT (**a**) and (5,5) SWCNT (**b**) calculated by B3LYP/6-31G*.

internal walls. The adsorption on the internal wall of (5,0) nanotube is the chemical adsorption and on the external wall of (5,0) and internal and external walls of (5,5) nanotubes are the physical adsorption. For these systems, the binding energy of the target gas analytes is low so that the analyte only fast desorbs from the CNTs after the sensor is exposed to an analyte-free atmosphere.

The lowest of energy gap is achieved in the process of $H_2S$ adsorption on the external wall of (5,5) nanotube. The energy gap is increased after the interaction of $H_2S$ on the internal and is decreased for external wall of (5,5) and (5,0) nanotubes. The lowest of HOMO and LUMO energies is obtained in the process of the adsorption on the external wall of (5,0) nanotube.

### $H_2S$ rotation on the nanotubes

$H_2S$ molecule rotation in two kinds of the horizontal and the vertical rotation relative to the axes of nanotubes have been shown in Figure 2. The effect of the internal and external adsorption of SWCNTs on the adsorption energy has been studied during these rotations at 30°, 60°, 90°, 120°, 150°, and 180° angles. The $H_2S$ molecule rotations are classified as follows:

1. Rotations 1a and 2a denote the rotations on the inside wall of (5,0) nanotube in the vertical and horizontal directions to the nanotube, respectively.
2. Rotations 1b and 2b indicate the rotations on the outside wall of (5,0) nanotube in the vertical and horizontal direction to the nanotube, respectively.

**Table 3 Partial charge differences on the interaction of atoms of the (5,0) nanotubes**

| Rotation | θ | $E_{ads}^{BSSE}$ | $E_{gap}$ | Dipole moment (μ) | ΔS | $\Delta H_1$ | $\Delta H_2$ | ΔC |
|---|---|---|---|---|---|---|---|---|
| **1a** | 0 | 2.0323 | 0.8106 | 3.7246 | 1.8604 | 0.0518 | 0.3105 | −0.0526 |
| | 30 | 0.7675 | 0.8432 | 2.4031 | 1.1786 | 0.0601 | −0.0204 | −0.0492 |
| | 60 | 0.5532 | 1.5477 | 1.5205 | 0.9563 | 0.0316 | −0.0273 | −0.0484 |
| | **90** | **0.5436** | **1.7218** | **0.8725** | **0.9569** | **0.0219** | **−0.0490** | **−0.0470** |
| | 120 | 0.8768 | 1.3437 | 0.6970 | 1.2709 | 0.0520 | −0.0520 | −0.0557 |
| | 150 | 1.3167 | 0.9438 | 2.5039 | 1.9173 | −0.0187 | −0.1076 | −0.0465 |
| | 180 | 2.3564 | 0.9765 | 2.3516 | 2.0999 | −0.0369 | −0.1650 | −0.0381 |
| **2a** | 0 | 2.3934 | 0.7997 | 0.4716 | 1.6957 | 0.0255 | −0.2562 | −0.1755 |
| | 30 | 0.8230 | 0.7698 | 1.8233 | 1.0823 | −0.0573 | 0.0392 | −0.1978 |
| | 60 | 0.5452 | 1.6538 | 1.2808 | 0.9696 | 0.0214 | −0.0537 | −0.0470 |
| | **90** | **0.5436** | **1.7218** | **0.8725** | **0.9569** | **0.0219** | **−0.0490** | **−0.0470** |
| | 120 | 0.7564 | 0.7235 | 3.4565 | 1.2828 | 0.0098 | 0.0054 | −0.0656 |
| | 150 | 1.9732 | 1.4498 | 1.9494 | 2.0339 | −0.1316 | −0.1698 | −0.0488 |
| | 180 | 3.9945 | 1.5123 | 2.7856 | 1.7721 | 0.0207 | 0.0835 | −0.0479 |
| **1b** | **0** | **−0.0027** | **1.7212** | **1.7648** | **−0.0129** | **0.0085** | **−0.0020** | **0.0000** |
| | 30 | 0.0018 | 1.7163 | 1.0973 | −0.0062 | 0.0110 | −0.0063 | 0.0035 |
| | 60 | −0.0015 | 1.7190 | 1.7782 | −0.0130 | 0.0085 | −0.0018 | −0.0002 |
| | 90 | −0.0011 | 1.7190 | 1.7894 | −0.0113 | 0.0071 | 0.0029 | −0.0040 |
| | 120 | −0.0009 | 1.7190 | 1.7335 | −0.0082 | 0.0031 | 0.0051 | −0.0023 |
| | 150 | −0.0007 | 1.7199 | 1.6803 | −0.0064 | 0.0006 | 0.0058 | −0.0015 |
| | 180 | −0.0005 | 1.7201 | 1.5586 | −0.0048 | −0.0009 | 0.0056 | −0.0012 |
| **2b** | 0 | 0.1056 | 1.4606 | 1.3541 | 0.1030 | 0.0388 | −0.0043 | −0.1292 |
| | 30 | 0.0035 | 1.7199 | 1.4269 | −0.0014 | 0.0047 | −0.0038 | −0.0219 |
| | 60 | −0.0015 | 1.7180 | 1.7418 | −0.0128 | 0.0084 | −0.0020 | −0.0005 |
| | **90** | **−0.0027** | **1.7212** | **1.7648** | **−0.0129** | **0.0085** | **−0.0020** | **0.0000** |
| | 120 | −0.0012 | 1.7207 | 1.9949 | −0.0123 | 0.0077 | −0.0029 | 0.0017 |
| | 150 | 0.0018 | 1.7163 | 2.1979 | −0.0033 | 0.0001 | −0.0036 | 0.0011 |
| | 180 | 0.0521 | 1.6946 | 1.9875 | 0.0613 | 0.0161 | −0.0141 | 0.0004 |

Rotation angle, θ, BSSE corrected adsorption energy, $E_{ads}^{BSSE}$(in Hartree), gap energy (in eV), dipole moment, $\mu$, (in Debye), and the difference partial natural charges on S, $H_1$, $H_2$ and C atoms (ΔS, $\Delta H_1$, $\Delta H_2$, and ΔC in esu) of the internal (a) and external (b) of (5,0) SWCNT-$H_2S$ molecule, vertical rotation (Figure 1) and horizontal rotation (Figure 2) calculated by B3LYP/6-31G*. BSSE, basis set superposition errors.

3. Rotations 1c and 2c represent the rotations on the inside wall of (5,5) nanotube in the vertical and horizontal direction to the nanotube, respectively.
4. Rotations 1d and 2d denote the rotations on the outside wall of (5,5) nanotube in the vertical and horizontal direction to the nanotube, respectively.

The origin of rotation angles for 1a, 2a, 1c, 2c, 2b, and 2d rotations is at 90°, and for 1b and 1d rotations is at 0°. The basis set superposition errors (BSSE) have been estimated for the counterpoise correction [35] and their effects on the energy changes during the rotation of $H_2S$ molecule inside and outside nanotubes have been calculated. This effect is much low for any considerations. It confirms the convenience of the chosen bases set. Based on the calculations, the most adsorption situations of $H_2S$ is at 90° for 1a, 2a, 2b, 1c, 2c, and 2d rotations and is at 0° for 1b and 1d rotations. The most favorable adsorption distance of $H_2S$ molecule on the external surface of (5,0) and (5,5) nanotubes is shown in Figure 3, where the distances from the external wall are 2.6 and 2.8 Å, respectively.

### NBO calculations

Gases absorption often changes the electronic properties of nanotubes. The environmental sensitivity can be useful in the detection of gas and making of gas sensors. Therefore, NBO calculations for all the rotations in order to calculate the charge difference before and after adsorption of $H_2S$ molecule on nanotubes have been performed.

**Table 4 Partial charge differences on the interaction of atoms of the (5,0) nanotubes**

| Rotation | θ | $E_{ads}^{BSSE}$ | $E_{gap}$ | Dipole moment (μ) | ΔS | $\Delta H_1$ | $\Delta H_2$ | ΔC |
|---|---|---|---|---|---|---|---|---|
| **1c** | 0 | 0.2137 | 1.6456 | 0.7476 | 0.0838 | −0.0010 | −0.0084 | −0.0345 |
| | 30 | 0.1147 | 1.7082 | 0.3385 | 0.0071 | −0.0076 | −0.0077 | −0.0139 |
| | 60 | 0.0701 | 1.7204 | 0.3942 | 0.0074 | −0.0098 | −0.0077 | −0.0057 |
| | **90** | **0.0442** | **1.7109** | **0.4002** | **−0.0151** | **0.0044** | **−0.0007** | **0.0121** |
| | 120 | 0.0489 | 1.7190 | 0.4189 | −0.0005 | −0.0035 | −0.0048 | 0.0008 |
| | 150 | 0.1209 | 1.7218 | 0.4131 | −0.0114 | 0.0011 | 0.0065 | 0.0020 |
| | 180 | 0.3319 | 1.4987 | 0.8966 | 0.3070 | 0.0061 | −0.0731 | 0.0036 |
| **2c** | 0 | 1.4636 | 0.7398 | 2.5268 | 0.7562 | 0.0852 | −0.1701 | 0.0065 |
| | 30 | 0.2162 | 1.7082 | 0.5222 | −0.0065 | −0.0162 | −0.0025 | 0.0131 |
| | 60 | 0.2080 | 1.7000 | 0.4170 | 0.0190 | 0.0003 | −0.0202 | 0.0077 |
| | **90** | **0.0442** | **1.7109** | **0.4002** | **−0.0151** | **0.0044** | **−0.0007** | **0.0121** |
| | 120 | 0.2352 | 1.7190 | 0.6128 | −0.0317 | 0.0235 | −0.0231 | 0.0034 |
| | 150 | 0.9334 | 0.7752 | 2.6623 | 0.6748 | −0.0152 | −0.0088 | 0.0070 |
| | 180 | 6.1295 | 1.0581 | 1.8876 | 2.1012 | −0.3712 | 0.2845 | −0.0061 |
| **1d** | **0** | **−0.0036** | **1.6997** | **1.8597** | **−0.0057** | **−0.0014** | **0.0033** | **−0.0183** |
| | 30 | −0.0033 | 1.7000 | 1.8483 | −0.0060 | −0.0007 | 0.0032 | −0.0169 |
| | 60 | −0.0010 | 1.6984 | 1.5994 | −0.0044 | 0.0010 | 0.0030 | −0.0129 |
| | 90 | 0.0330 | 1.6973 | 1.2374 | 0.0097 | −0.0001 | 0.0029 | −0.0082 |
| | 120 | 0.0290 | 1.6978 | 1.0797 | −0.0004 | 0.0024 | −0.0024 | −0.0025 |
| | 150 | −0.0013 | 1.6967 | 1.7147 | −0.0049 | 0.0037 | 0.0010 | −0.0033 |
| | 180 | −0.0016 | 1.6970 | 1.5341 | −0.0039 | 0.0040 | −0.0002 | −0.0035 |
| **2d** | 0 | 0.0315 | 1.6916 | 3.0257 | 0.0152 | −0.0162 | −0.0112 | −0.0275 |
| | 30 | 0.0049 | 1.6967 | 2.5708 | −0.0038 | −0.0016 | 0.0007 | −0.0159 |
| | 60 | −0.0015 | 1.6989 | 2.2489 | −0.0078 | 0.0010 | 0.0032 | −0.0172 |
| | **90** | **−0.0036** | **1.6997** | **1.8597** | **−0.0057** | **−0.0014** | **0.0033** | **−0.0183** |
| | 120 | 0.0146 | 1.6978 | 1.2982 | −0.0032 | −0.0032 | 0.0031 | −0.0179 |
| | 150 | −0.0033 | 1.6976 | 0.8383 | −0.0018 | −0.0040 | 0.0039 | −0.0156 |
| | 180 | 0.0134 | 1.6976 | 0.9206 | −0.0005 | −0.0043 | 0.0090 | −0.0123 |

Rotation angle, θ, BSSE corrected adsorption energy, $E_{ads}^{BSSE}$ (in Hartree), gap energy (in eV), dipole moment, $\mu$, (in Debye), and the difference partial natural charges on S, $H_1$, $H_2$, and C atoms (ΔS, $\Delta H_1$, $\Delta H_2$ and ΔC, in esu) of the internal (c) and external (d) of (5,5) SWCNT-$H_2S$ molecule, vertical rotation (1) and horizontal rotation (2), calculated by B3LYP/6-31G*. BSSE, basis set superposition errors.

The partial charge differences on the interaction of atoms including sulfur atom, hydrogen atoms and nearest carbone atom of interaction zoon of the (5,0) and (5,5) nanotubes in the presence of $H_2S$ molecule in the vicinity of internal and external walls for all rotations have been shown in Tables 3 and 4. They represent the change in the electronic structure of nanotube. They can be used as a response of the adsorption in the sensor equipments.

## Conclusions

$H_2S$ molecule adsorption on the internal and external wall of (5,0) nanotube is both chemical and physical adsorption. The absorption on both internal and external walls of (5,5) nanotube is physical absorption. Based on the calculations, the most adsorption situations of $H_2S$ occur at 90° during the parallel and vertical rotations of the $H_2S$ molecule to the main axes inside of the nanotube. This situation is the same as the parallel rotation outside of the nanotube. The vertical rotation outside of the nanotube has the most adsorption energy at 0°. The most favorable adsorption distances from the molecule to external of (5,0) and (5,5) SWCNTs are 2.6 and 2.8 Å, respectively. The results of the thermodynamic quantities certifies no simultaneous $H_2S$ adsorption process, while the NBO analysis shows the change in the electronic structure of nanotubes which may be suitable fabricating sensors in providing an immediate feedback on the environment by SWCNTs. In these sensors, the electrical properties of nanostructures are dramatically changed when exposed to the target gas analytes and the analyte desorbs from the SWCNTs after the sensor is exposed to an analyte-free atmosphere.

#### Competing interests

The authors declare that they have no competing interests.

#### Authors' contributions

MO conceived of the study, participated in the design of the study and in the sequence alignment and drafted the manuscript. MG participated in drafting the manuscript and its design and coordination. HHA participated for his assistance and efforts for optimizing the 3D geometry of the structures studied. All authors read and approved the final manuscript.

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