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Research Article

Electronic Properties of Boron and Silicon Doped (10, 0) Zigzag Single-Walled Carbon Nanotube upon Gas Molecular Adsorption: A DFT Comparative Study

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We have performed a comparative study of nine predominant gas molecules (H_2, H_2O, O_2, CO, CO_2, NO, NO_2, NH_3, and CH_3OH) adsorption property on the top surface of the (10, 0) zigzag single-walled pristine Carbon nanotube (C-CNT), Boron doped carbon nanotube (B-CNT), and Silicon doped carbon nanotube (Si-CNT) are investigated by using density functional theory (DFT) computations to exploit their potential applications as gas sensors. For the first time, we calculated the optimal equilibrium position, absorption energy (E_{ad}), and density of states (DOS) of the considered gas molecules adsorbed on the open end of zigzag single-walled (10, 0) B-CNT and Si-CNT. Our first principle calculations demonstrate that the B-CNT and Si-CNT adsorbent materials are able to adsorb the considered gas molecules with variety of adsorption energy and their electronic structure dramatic changes in the density of states near the Fermi level. The obtained comparative DFT studies results are useful for designing a high-fidelity gas sensor materials and selective adsorbents for a selective gas sensor.

1. Introduction

Gas molecular adsorption in nanostructures is an important issue for both fundamental research and technical application. In recent years, carbon nanotubes have been intensively studied due to their importance as building blocks in nanotechnology. The special geometry and unique properties of carbon nanotubes offer great potential applications, such as nanoelectronic devices, fuel cell, energy storage, chemical probes and biosensors, field emission display, and gas sensor [1–4]. Carbon nanotubes (CNTs) have the potential to be developed as a new gas sensing material due to their inherent properties such as their small size, great strength, high electrical and thermal conductivity, high surface-to-volume ratio, and hollow structure of nanomaterials. As a result, it is possible to create a miniaturized sensor, which can lead to low power consumption, lighter, and low cost. Therefore, CNTs-based gas sensors and their mechanisms have been widely studied recently. Different kinds of nanotubes have been investigated for gas molecules adsorption, such as carbon nanotubes (CNTs) [5–15], boron nitride nanotubes (BNNTs) [16–22], boron doped nanotubes [23–27], silicon carbide nanotubes [28–46], zinc oxide nanotube, TiO_2 nanotube, tungsten carbide nanotube, and MgO nanotube [47]. Meanwhile, the efficiency of gas adsorption on pristine carbon nanotubes can be enhanced by doping process [16–46].

Doping (heteroatom substitution) is also a promising approach to enable single-walled carbon nanotubes (SWCNTs) to detect gas molecules as well as organic chemicals and biological substances, since the adsorption capability of SWCNTs can be improved through introducing heteroatom impurities (such as boron, nitrogen, silicon, zinc, and titanium) and forming active sites in tube walls. In the literature, a lot of papers briefly discussed gas molecules adsorption property of boron doped carbon nanotube and nitrogen doped carbon nanotube. Further, the potential of silicon doped carbon nanotube (Silicon carbide nanotube) gas molecules adsorption property has to be investigate for various small gases such as H_2, H_2O, O_2, CO, CO_2, NO, NO_2, NH_3, and CH_3OH. The recently synthesized silicon carbide (SiC) nanotube [44, 45] has been found to be a semiconducting material and is of great technological interest

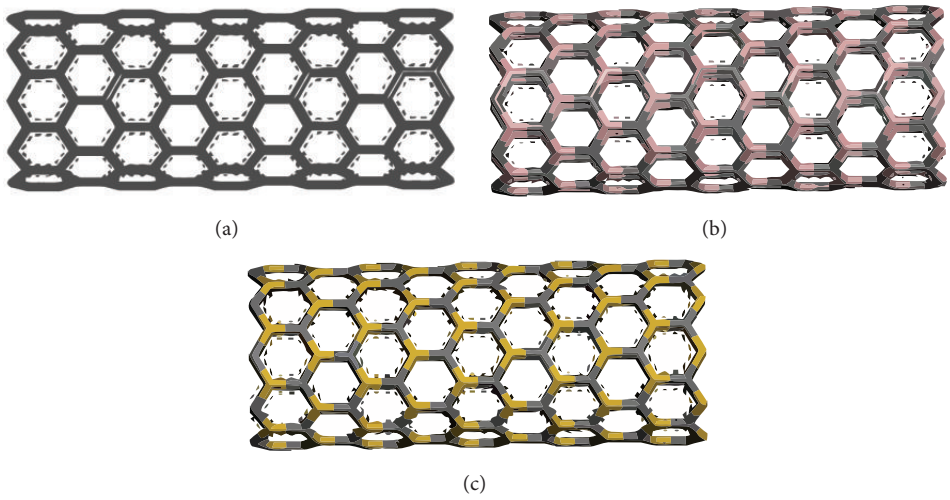


Figure 1: Gas molecules adsorbents model (a) (10, 0) zigzag single-walled Pristine Carbon nanotube, (b) (10, 0) zigzag single-walled Boron doped carbon nanotube (B-CNT), and (c) (10, 0) zigzag single-walled silicon doped carbon nanotube (Si-CNT).

for devices designed to operate at high temperatures, high power, and in harsh environments. An attractive point is that SiC nanotube has higher reactivity than carbon nanotube (CNT) or boron nitride nanotube (BNNT) due to its great polarity [42, 43]. Obviously, these unique properties of SiC nanotube are the key advantages for its applications to the building blocks in the fabrication of electronic nanodevices and chemical adsorbents.

Exploring the electronic properties of SiC nanotubes upon considered gas molecule absorption condition is very helpful for widening their practical applications such as gas sensor, and many routes have been addressed to evaluate the changes of their properties. Very recently, Gao et al. investigated theoretically the interaction between NO_2 molecule and SiC nanotube [35]. They reported that a single NO_2 molecule can be chemically adsorbed on the outer surface of SiC nanotube with a relatively large adsorption energy (~1.0 eV), and the electronic properties are modified by the NO_2 adsorption. Followed by CO, NO, and O_2, gas molecules adsorption property on silicon carbide nanotube is investigated theoretically by [30–46]. However, to our knowledge, no experimental or theoretical investigation has been reported on the adsorption of H_2, H_2O, CO, NH_3, and CH_3OH on the surfaces of silicon doped carbon nanotube (Si-CNT). Such a study has been done in this paper.

In this paper, we focus on the interaction behavior of important classes of molecules (H_2, H_2O, O_2, CO, CO_2, NO, NO_2, NH_3, and CH_3OH) with C-CNT, B-CNT and Si-CNT being studied extensively by DFT method. The overall aim of this study is to provide the fundamental insight into the molecular interactions between these common gaseous and our proposed adsorbates B-CNT and Si-CNT models. The adsorption energy (E_{ad}), binding distance (BD), and electronic structure of the considered gas molecular species are calculated. This information is ultimately necessary for the molecular design of new adsorbents and sensing materials. Our first-principle calculations demonstrate that the proposed models of B-CNT and Si-CNT exhibit a variety of adsorption interactions and their electronic structure dramatic changes in the density of states near the Fermi level with the considered gas molecule being probed. This information can be used to guide experimental synthesis, depending upon the requirements of the specific gas sensor application.

2. Computational Methods

In the present work, adsorption behaviors of the nine predominate gas molecules are studied by using the C-CNT, B-CNT and Si-CNT, representative models of open edge (10, 0) zigzag single-walled nanotubes (SWNTs) with optimized molecular orientations. A primary (10, 0) C-CNT containing 160 carbon atoms with length of 17.04 Å is chosen for the purpose. Since the exact distribution of boron atoms on the nanotube was still unknown, for the B-CNT (10, 0) structure, we distributed ten carbon atoms in the primary C-CNT (10, 0) supercell which were substituted by B atoms with only one constraint: boron atoms could not occupy the positions of their nearest neighbors on the hexagonal carbon structure. The structural verification and stability of the B-CNT (10, 0) models employed in this work have been described elsewhere [23–27]. The Si-CNT (10, 0) structure also constructed C80Si80 atomic configuration in a supercell. The adsorbents nanotube models are shown in Figures 1(a), 1(b), and 1(c), respectively. One-dimensional periodic boundary condition are applied along the tube axis. The number of carbon layers along the tube axis is chosen such that the absolute value for the total charge approaches zero and the total energy do not change as the number of layers increased. For all the tubes, one gas molecule per unit cell is considered in the tube axis direction. Density functional theory (DFT) has been extensively used for the calculation of adsorption energy and density of states (DOS) properties of individual pristine carbon nanotube (C-CNT), boron doped carbon nanotube (B-CNT), and silicon doped carbon nanotube (Si-CNT) on gas adsorption. The self-consistent field (SCF) electronic structure calculations are performed based on density functional theory

(DFT) with either localized basis (DMol) or plane-wave basis (CASTEP) [48]. The equilibrium geometry and adsorption energy are calculated by using the DMol program. The density functional is treated by the local density approximation (LDA) with exchange-correlation potential parameterized by [48]. The energy cutoff of the plane wave basis is chosen up to 760 eV. In this paper, we find out that the optimum adsorbates orientation, and optimum binding distance have been attempted in order to locate the lowest energy configuration of the adsorbate + tube system. The adsorption energy (E_{ad}) is defined as the difference between the energy of the SWCNT + molecule(s) system, minus the sum of the energies of the SWCNT and of the isolated molecule(s) in the same conditions. (Supercell size, k-points, etc.). Negative values of E_{ad} denote an exothermic adsorption process. We calculated adsorption energy (binding energy) of the system as a function of the distance between the gas molecule and the surface of the wall for various orientations. The adsorption energy E_{ad} is calculated according to the expression (1) as follows:

$$E_{ad} = \left(E_{tube} + E_{gas}\right) - E_{tube\text{-}gas}. \quad (1)$$

It should be noted that calculation of the charge on atoms is quite difficult. However, the charge transfer between the molecule and the nanotube is calculated from the charge difference of each atom before and after molecule absorption, which should be independent of the method used, although, in practice, some minor deviations may exist.

3. Results and Discussions

It is essential to understand the adsorption behavior of several potentially-important molecular species. Thus, the adsorption energy (E_{ad}), binding distance (BD), electronic band structure, and density-of-states (DOS) of the considered gas molecular species are calculated, and this information can be used to clearly define the adsorption nature of these molecules on the C-CNT, B-CNT, and Si-CNT adsorbents material. The most stable configurations for the gas adsorbates based on Si-CNT (our choice of interested adsorbent model) are displayed in Figure 2. Like that, the most stable configurations for the gas adsorbates based on B-CNT are also chosen for our calculation, which is not shown here. The represented silicon carbide nanotube model consist of Si and C atomic structure. The calculated average Si–C bond length of these tubes is about 1.819 Å.

In the following subsections, the adsorption energies, optimum binding distance between the molecular, charge transfer (Q) between gas molecules and nanotube, electronic band structure, and total density of states of the (10, 0) zigzag single-walled C-CNT, B-CNT, and Si-CNT that interacted with the considered gas molecule species are discussed. To establish a well-defined comparative study, we have performed the calculations using unit cells of similar sizes and parameters.

3.1. Interaction between Gas Molecule and Adsorbates. The adsorption of H_2, H_2O, O_2, CO, CO_2, NO, NO_2, NH_3, and CH_3OH on C-CNT, B-CNT, and Si-CNT are calculated and can be characterized as physisorption and chemisorption, as indicated by the magnitude of adsorption energy (E_{ad}) and binding distance (BD). Table 1 summarizes our results on the optimum stable binding tube-molecule distance (BD), adsorption energy (E_{ad}), and charge transfer (Q) (positive Q means charge transfer from molecule to tube) for a considered gas molecules adsorption on the proposed representative model of (10, 0) zigzag single-walled nanotube. In general, all these gas molecules are weakly bounded to the pristine carbon nanotube and the tube-molecule interaction can be identified as physisorption. Most molecules studied (with exception of NO_2 and O_2) are charge donors with small charge transfer (0.01 to 0.04 electron per molecule) and weak binding (−0.2 eV). For O_2 and NO_2, both of which are charge acceptors, the charge transfer is not negligible. This is also reflected in their average adsorption energies. As it is known, pristine C-CNTs are rather inert and engage in only weak, van der Waals-type interactions with most molecules, due to their strong sp_2 bonding network. The binding of H_2 onto pristine CNT sidewalls are characterized as a physisorption interaction.

In contrast, our calculations show that the Boron doped carbon nanotube (B-CNT) exhibits significantly enhanced binding with H_2, the concede adsorption energy (E_{ad}), and binding distance (BD) between tube and molecules which are −0.89 eV and 1.83 Å. Our calculations indicate that CO, CO_2, and NO_2 are also strongly chemisorbed on B-CNT and concede an adsorption energy (E_{ad}) values of −2.33, −2.30, and −4.31 eV, respectively. In addition, O_2 and NO due to strong exothermic process, can atom both completely dissociate into individual atoms that concede large adsorption energy values of −8.64 and −7.24 eV per molecule, respectively. On the other hand, the adsorption of H_2O, CH_3OH, and NH_3 on B-CNT can be characterized as molecular chemisorption, as indicated by the average E_{ad} values. In particular, the binding strength of H_2O, CH_3OH, and NH_3 is found to increase with respect to their tendency to donate electrons and concede adsorption energy values of −1.19, −1.35, and −1.72 eV, respectively. The proposed model of silicon carbide nanotube (Si-CNT) also shows an improved chemisorbed adsorption energy as compared to pristine carbon nanotube but not with B-CNT. Our calculations indicate that O_2 and CH_3OH are strongly chemisorbed on Si-CNT as compared to the C-CNT and B-CNT. Si-CNT concede large adsorption energy values of −36.77 and −3.42 eV per molecule, respectively. On the other hand, the adsorption of H_2, H_2O, CO, CO_2, NO, NO_2, and NH_3 on Si-CNT concede lower adsorption energy values of −0.32, −0.45, −0.74, −0.63, −0.23, −1.45, and −0.24 per molecule, respectively, as compared to B-CNT. But while comparing with C-CNT, Si-CNT shows a higher adsorption energy with respect to all the gas molecules considered. In Table 1, we show the large adsorption energy values for each gas molecules in a bold face letter. The comparative DFT study result shows that the B-CNT and Si-CNT adsorbent materials which show a strong accept or donor of electron with respect to specific gas molecules, and it could be favor adsorbates for various specific gas sensor applications.

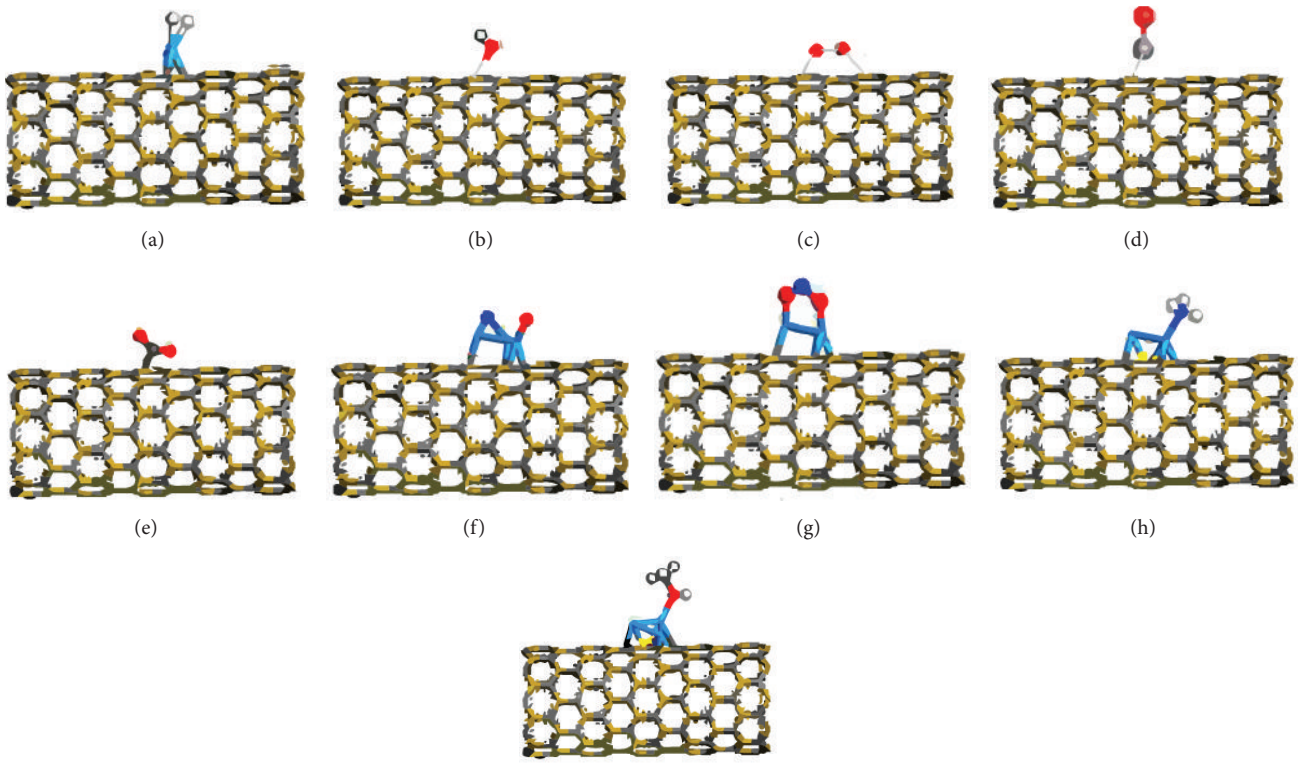


Figure 2: Optimized stable configurations of the Si-CNT nanotube adsorbates with considered gas molecules: (a) H_2, (b) H_2O, (c) O_2, (d) CO, (e) CO_2, (f) NO, (g) NO_2, (h) NH_3, (i) CH_3OH.

Table 1: Adsorption energy (E_{ad}) per molecule, binding distance (BD) and charge transfer (Q) (positive Q means charge transfer from molecule to tube) for a considered gas molecules on the specified adsorbent model.

Adsorbents model		H_2	H_2O	O_2	CO	CO_2	NO	NO_2	NH_3	CH_3OH
(10, 0) Pristine carbon nanotube (C-CNT)	E_{ad} (eV)	−0.12	No binding	−0.51	No binding	−0.97	−0.041	−0.78	−0.15	−3.35
	BD (Å)	2.81		2.32		3.20	3.46	1.93	2.99	1.96
	Q (e)	0.014		−0.13		0.018	0.009	−0.064	0.033	0.013
(10, 0) Boron doped carbon nanotube (B-CNT)	E_{ad} (eV)	**−0.89**	**−1.19**	−8.64	**−2.33**	**−2.20**	**−7.24**	**−4.31**	**−1.72**	−1.35
	BD (Å)	1.83	2.24	1.76	2.03	2.02	1.75	1.96	2.26	2.19
	Q (e)	0.12	0.16	0.21	0.19	0.18	0.20	0.21	0.16	0.13
(10, 0) Silicon carbide nanotube (Si-CNT)	E_{ad} (eV)	−0.32	−0.45	**−36.77**	−0.74	−0.63	−0.23	−1.45	−0.24	**−3.42**
	BD (Å)	2.05	2.62	1.72	1.93	1.82	2.51	2.01	2.87	1.98
	Q (e)	0.10	0.11	0.23	0.17	0.12	0.08	0.18	0.09	0.20

3.2. Electronic Properties of Gas Adsorbates upon Molecule Adsorption. To further understand the adsorption properties of considered gas molecules on the proposed representative model and the gas adsorbed nanotube electronic structure are calculated in terms of electronics band structure and density of state (DOS) for the B-CNT and Si-CNT system. In this paper, our choice of interested models are B-CNT and Si-CNT. In this section, we discuss the electronic band structure and density of state of adsorbates B-CNT and Si-CNT upon each gas molecule adsorption condition. Before that, we calculated the electronic band structure and density of state of the proposed B-CNT and Si-CNT adsorbate model without gas molecule adsorption condition. The electronic band structure and density of state of adsorbate nanotubes are shown in Figures 3, 6(a), 6(b), and 6(c), respectively. There Fermi energy (E_F) levels are denoted by dashed line and their respective values are $E_F = 1.3$ ev and $E_F = -4.36$.

Figures 4 and 5 show the electronic band strucutre for the considered gas molecule adsorbed on the B-CNT and Si-CNT systems. Figures 7 and 8 show the electronic density of states (DOS) for the considered gas molecule adsorped on the B-CNT and Si-CNT systems. It can be seen that the DOS near the Fermi level (E_F) is affected by the adsorption of considered gas molecule in the B-CNT and Si-CNT surface.

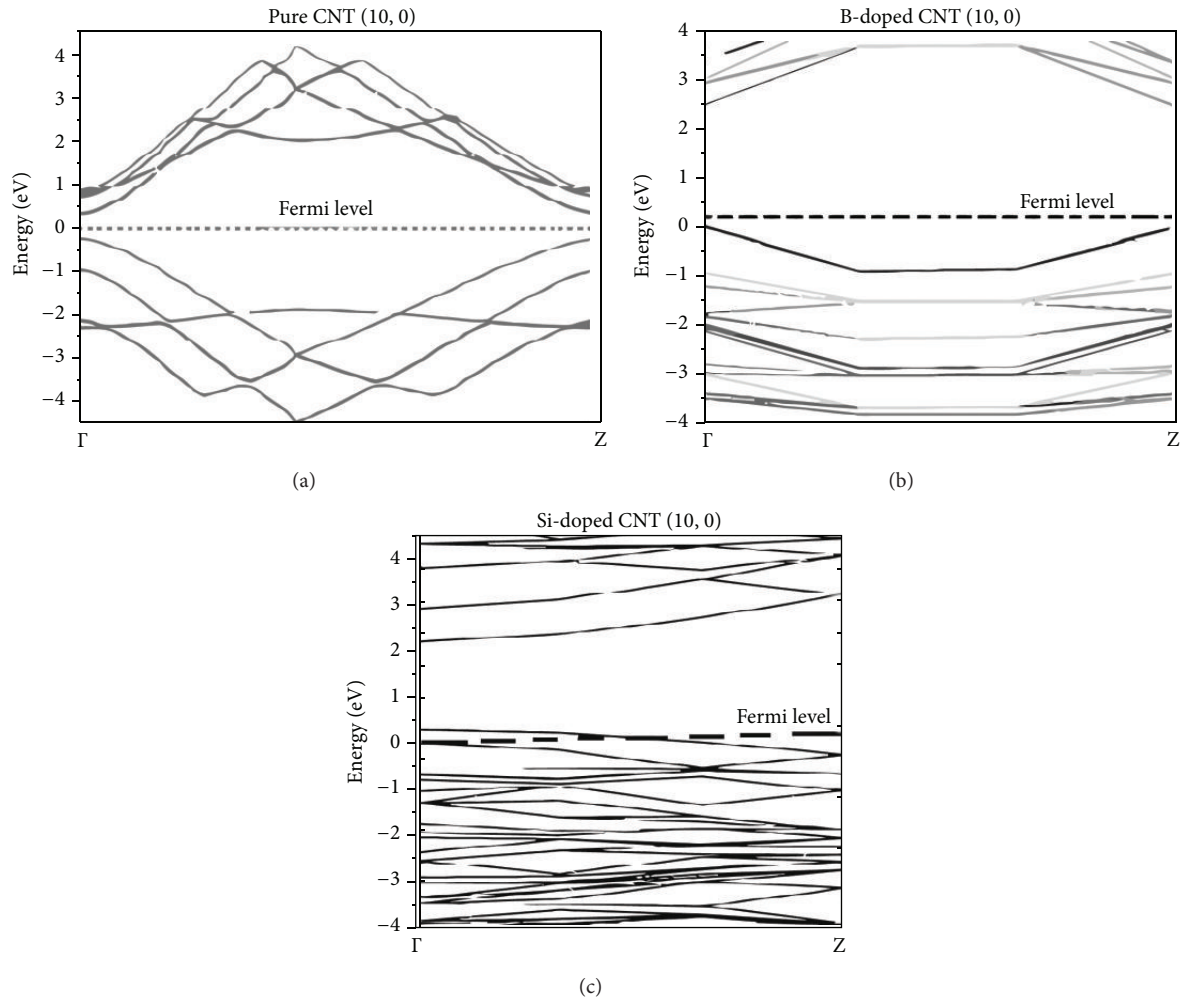


Figure 3: Band structures of the (10, 0) indexed: (a) pure carbon nanotube, (b) boron doped carbon nanotube (B-CNT), and (c) silicon doped carbon nanotube (Si-CNT) without gas molecules adsorption condition. The dashed lines indicate the position of Fermi level.

Table 2: Fermi energy (E_F) of the B-CNT and Si-CNT models with and without adsorption of considered gas molecules.

Adsorbents model	Fermi energy E_F (eV)								
	H_2	H_2O	O_2	CO	CO_2	NO	NO_2	NH_3	CH_3OH
(10, 0) Boron doped carbon nanotube (B-CNT)									
Without gas molecule adsorption					1.3				
With gas molecule adsorption	−7.3	−5.9	−8.5	−8.2	−9.7	−7.5	−8.4	−8.6	−8.2
(10, 0) Silicon carbide nanotube (Si-CNT)									
Without gas molecule adsorption					−4.36				
With gas molecule adsorption	−2.5	−3.5	−3.6	−3.1	−3.2	−3.5	−3.2	−4.1	−2.2

The Fermi energy (E_F) values of the gas adsorped adsorbent nanotube are summarized in Table 2. From the comparison, we can also see that the DOS of the B-CNT and Si-CNT where the gas molecule is adsorbed shifts down or upward by some amount of eV in comparison with a bare (10, 0) B-CNT and Si-CNT. This substantial shift can be explained by the reduction in effective Coulomb potential due to the charge transfer. On the other hand, the difference in the Fermi level of the B-CNT and Si-CNT clearly shows a charge transfer between the considered gas molecule and B-CNT and Si-CNT system in the adsorption process. From the DFT comparative study, we recommend (based on the adsorption energy between the considered gas molecules and adsorbents nanotube model) a high sensitive specified adsorbates nanotube model for the considered gas molecules shown in Table 3.

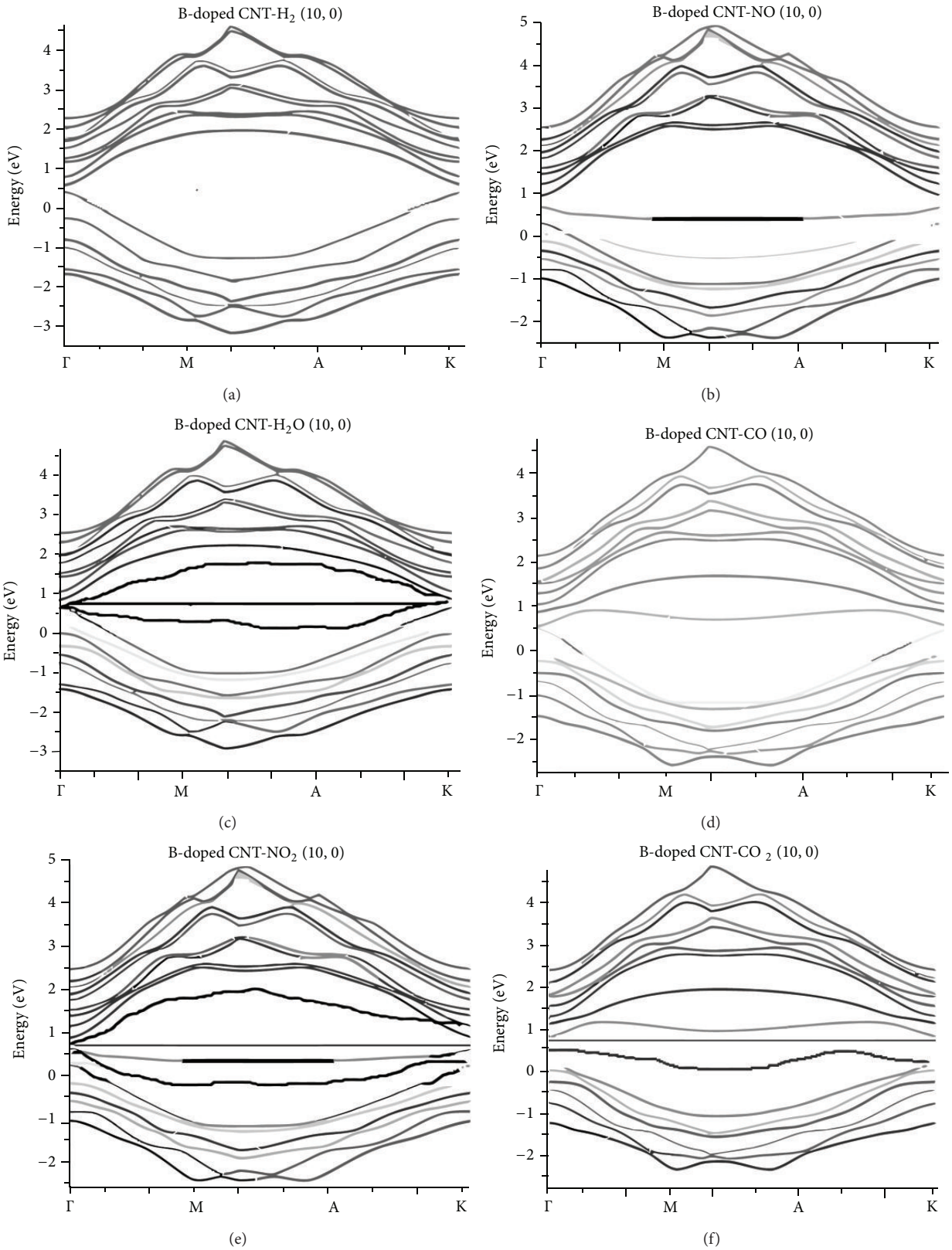


Figure 4: Electronic band structures for the (10, 0) boron doped CNT (B-CNT) adsorbates with considered gas molecules adsorption condition: (a) H_2, (b) NO, (c) H_2O, (d) CO, (e) NO_2, (f) CO_2.

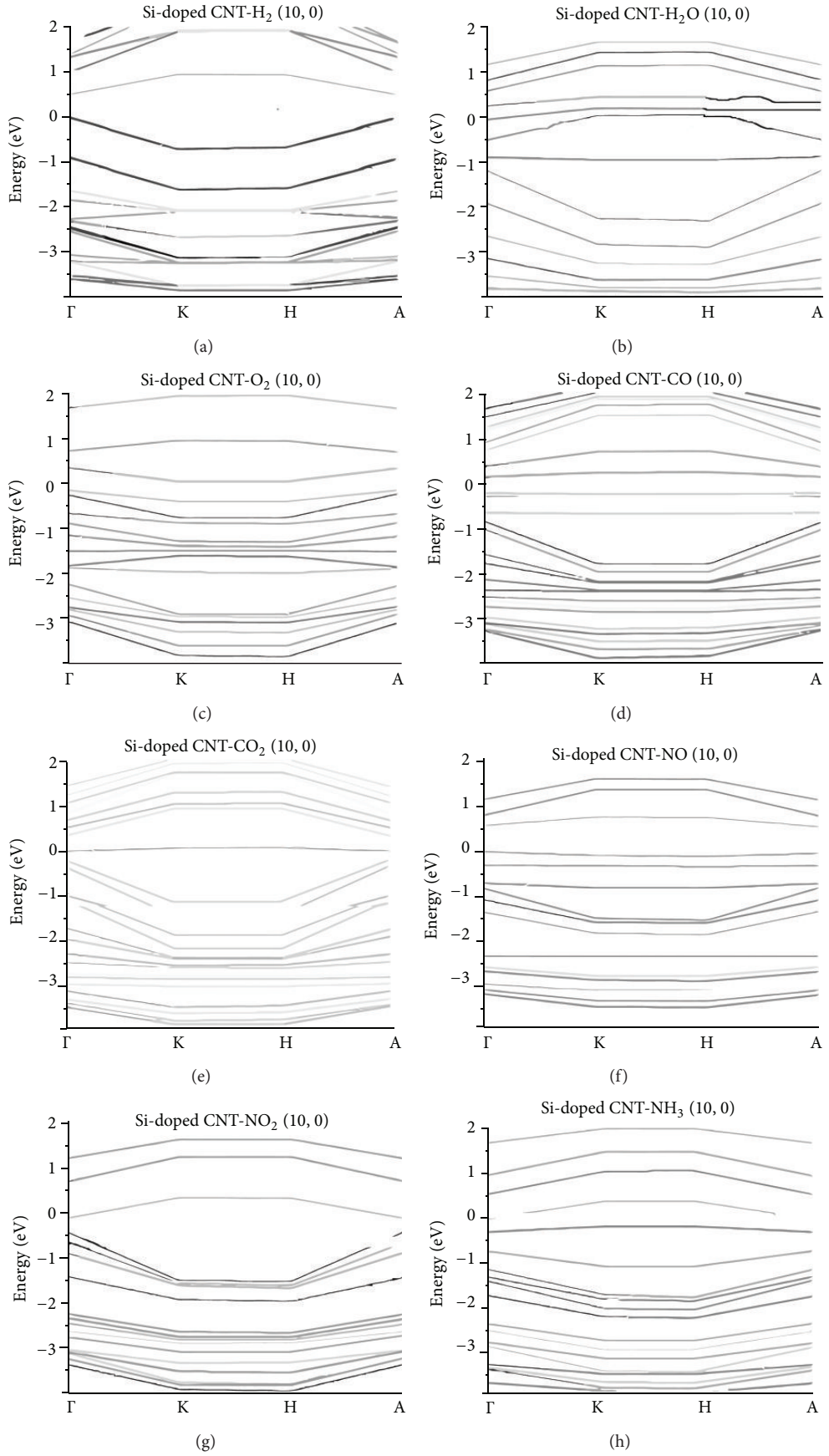
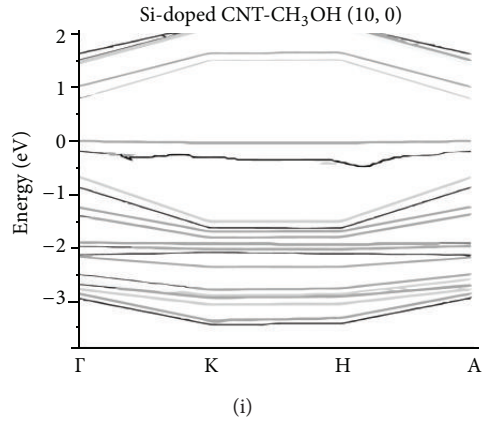


Figure 5: Continued.



(i)

Figure 5: Electronic band structures for the (10, 0) silicon doped CNT (Si-CNT) adsorbates with considered gas molecules adsorption condition: (a) H_2, (b) H_2O, (c) O_2, (d) CO, (e) CO_2, (f) NO, (g) NO_2, (h) NH_3, (i) CH_3OH.

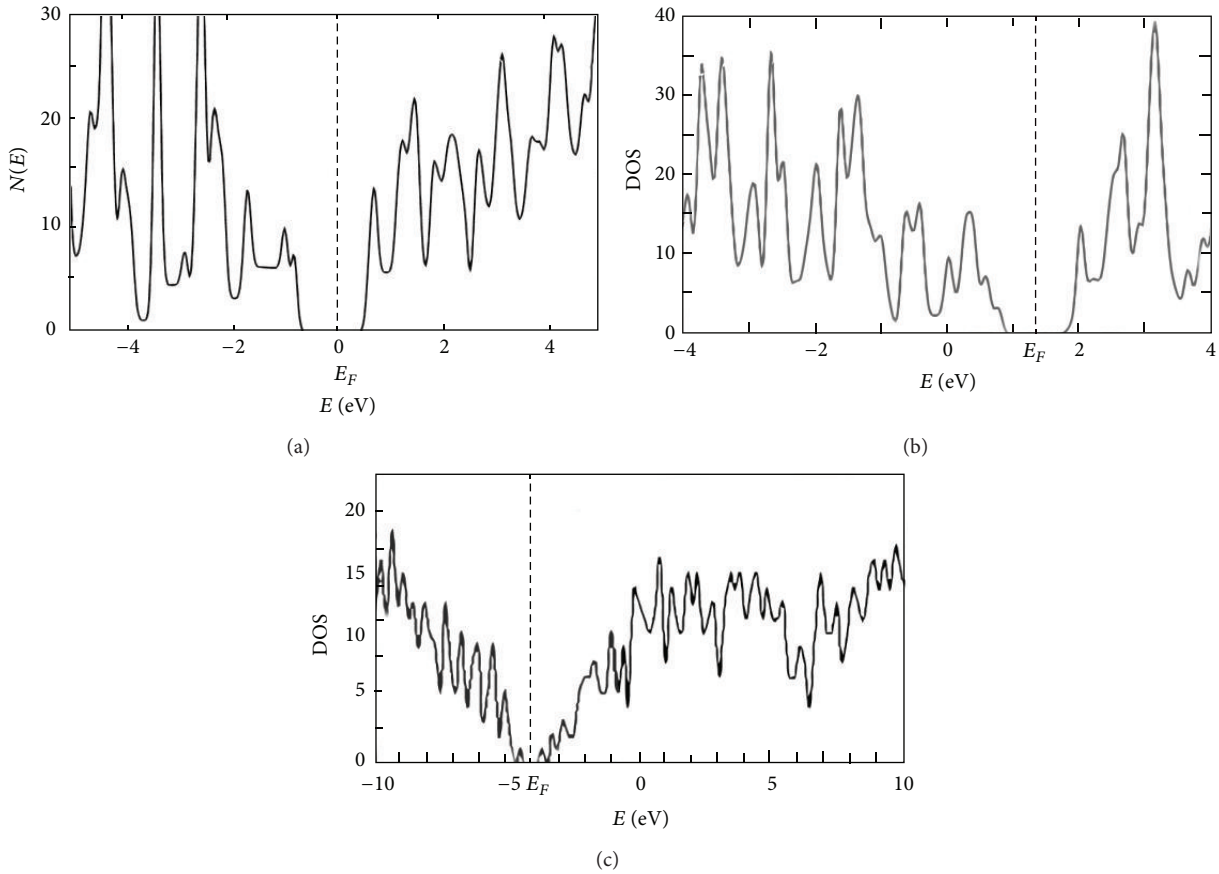


Figure 6: Electronic density of states of the adsorbents without gas molecule adsorption condition: (a) (10, 0) zigzag single-walled C-CNT, (b) (10, 0) zigzag single-walled B-CNT, and (c) (10, 0) zigzag single-walled Si-CNT.

4. Conclusion

We perform first-principle DFT studies on the adsorption of nine predominate gas molecules (H_2, H_2O, O_2, CO, CO_2, NO, NO_2, NH_3, and CH_3OH) on a C-CNT, B-CNT, and Si-CNT (10, 0) zigzag single-walled adsorbent nanotube material. We found that all molecules are weakly adsorbed on pristine carbon nanotube adsorbent with small binding energy, while they can be either charge donor or accepter of nanotube. Finally, we found that the B-CNT and Si-CNT adsorbents are highly chemisorption when exposed to NO, NO_2, and O_2, CH_3OH. The Si-CNT adsorbent also moderately adsorbs H_2, H_2O, CO, CO_2, and NH_3 gas molecules with binding strengths compared with B-CNT adsorbates. The electronic

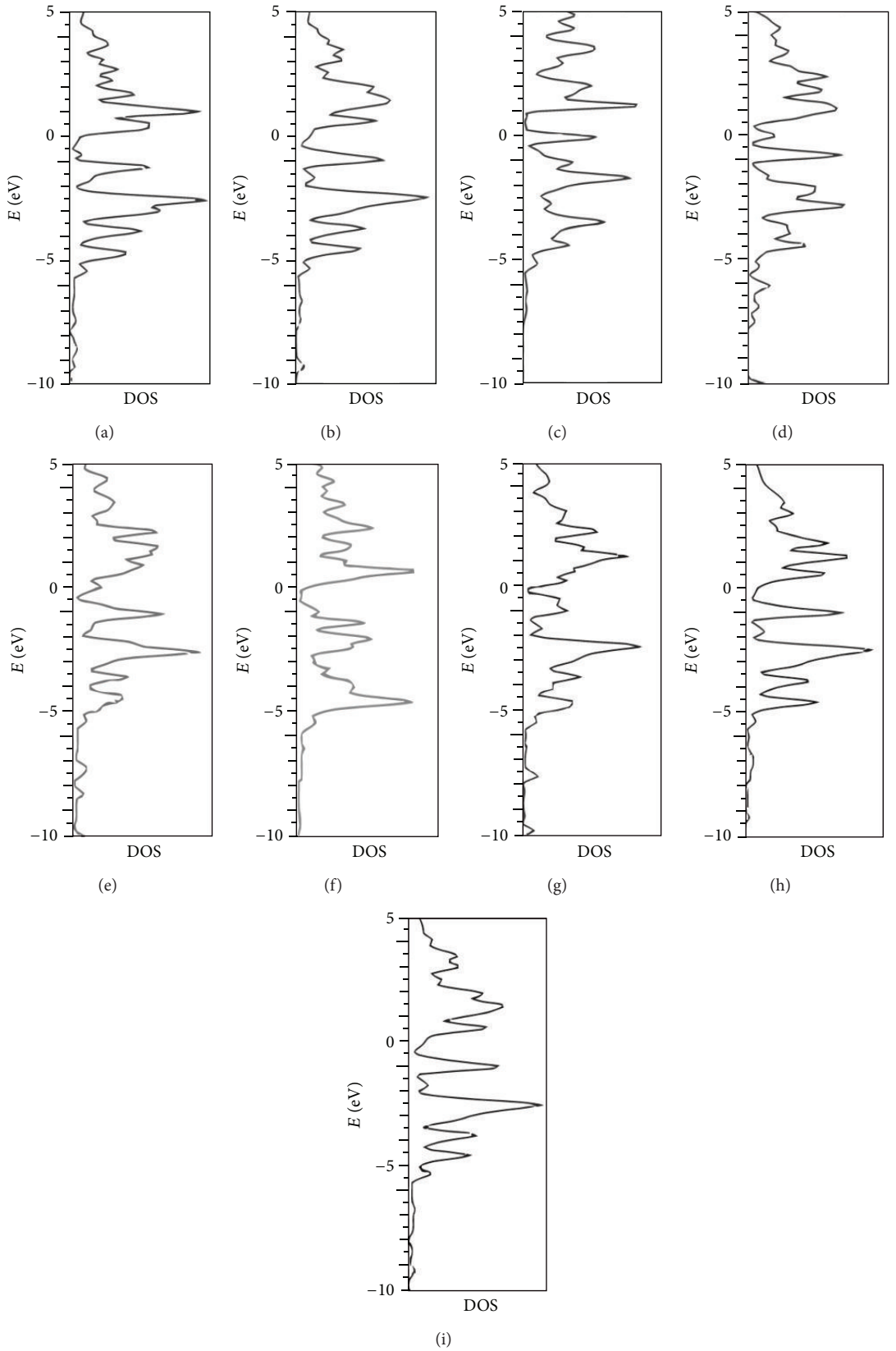


Figure 7: Electronic density of states (DOS) of the B-CNT adsorbates with considered gas molecules adsorption condition: (a) H_2, (b) H_2O, (c) O_2, (d) CO, (e) CO_2, (f) NO, (g) NO_2, (h) NH_3, (i) CH_3OH.

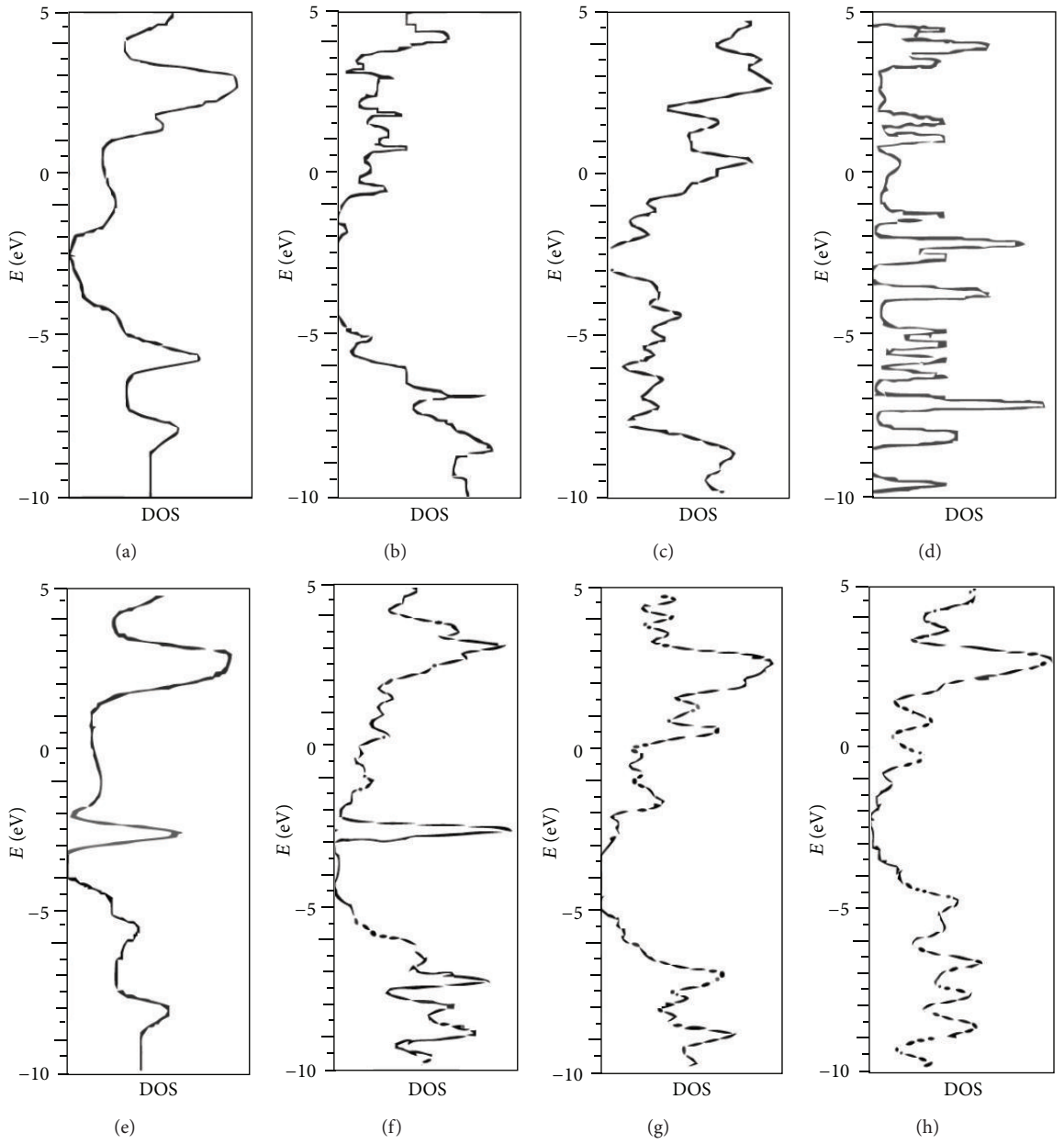


Figure 8: Electronic density of states (DOS) of the Si-CNT adsorbates with considered gas molecules adsorption condition: (a) H_2, (b) H_2O, (c) O_2, (d) CO, (e) NO, (f) NO_2, (g) NH_3, (h) CH_3OH.

Table 3: Recommendations for a high sensitive specified adsorbate model for considered gas molecules.

Gas molecules	Adsorption type	High sensitive adsorbate model
H_2, H_2O, NO, NO_2, CO, CO_2, and NH_3	Chemisorption	Boron doped carbon (B-CNT) nanotubes
O_2 and CH_2OH	Chemisorption	Silicon doped carbon (Si-CNT) nanotubes

band structure and DOS calculations of these systems show that the strong adsorption (chemisorption) of considered gas molecules is able to show dramatic changes in the density of states near the Fermi level. The quantum molecular dynamic (MD) simulation carried out at room temperature and results show that the B-CNT and Si-CNT adsorbent materials would be good candidates for gas sensor applications. Finally, the proposed methodology of designing gas sensors can be followed to fabricate reliable, sensitive, and selective nanotube sensors.

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