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First-Principles Study of Nanotube- Based Gases Sensors For O2, CL2, F2 and CO Detection: DFT/B3LYP Investigations

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ABSTRACT

Objective: *This study examines the sensing potential of carbon nanotubes (CNTs) for the adsorption of F2, O2, CL2, and CO molecules.* ***Method:*** *Investigations were conducted on the electronic properties, adsorption energy, and geometry optimization. The density functional theory at the B3LYP/631G level using the Gaussian 09W software package serves as the foundation for all of the computations.* ***Results:*** *The distance between the CNTS and CL2, O2, F2, and CO molecules determines the adsorption process. All of the structures also have different levels of chemical hardness and electron affinity. This indicates that, for such structures to be cations or anions, a higher energy was required to donate or accept an electron. The usage of CNTS as a nanosensor is confirmed by this study.* ***Novelty:*** *Because of their special properties, Carbon Nanotube (CNTs) have drawn a lot of attention. A variety of devices, including nanosensors, could make use of such CNTS properties. High sensitivity to unique gas molecules and quick response times make CNTS nanosensors ideal for critical applications. Recently, the theoretical investigation regarding gas adsorption across the outer surface of CNTS nanosensors has been deemed quite intriguing.*

INTRODUCTION

Another type of carbon is a 1D nanotube, which was initially identified by Ijma in the year 1991 when he found multi-walled carbon nanotubes (MWNT) in carbon-soot produced using the arc-discharge technique [1], [2]. He discovered single-walled nanotubes (SWNTs) approximately two years later [3]. Since then, researchers from all across the world have become interested in nanotubes [4]. In the last ten years, a great deal of research was done to uncover the special electrical, structural, mechanical, and chemical properties regarding CNTs as well as to investigate potential major uses for such cutting-edge materials [5], [6], [7].

Because of their significance as a building block in nanotechnology, CNTs were extensively investigated [8]. Energy storage, nanoelectronics devices, chemical probes and biosensors, and field emission displays are just a few of the many possible uses for CNTs' special geometry and exceptional chemical properties [9]. For both basic study and practical use of nanotubes, gas adsorption in CNTs and nanotube bundles is a crucial problem. The storage of hydrogen in materials depending on nanotubes was the subject of extensive theoretical and experimental research. Lately, there has been some interest in how the gas environment affects the electron properties of CNTs. The electrical conductivity regarding the semiconducting tubes is significantly altered by exposure to gas, such as CO. The electronic properties of small semiconducting nanotubes are significantly impacted by O2 adsorption [10], [11].

RESEARCH METHOD

The density functional theory (DFT) provides a rigorous mathematical basis for current ab initio simulation techniques [12], [13], [14], and [15]. The electronic structure problem is reduced to a self-consistent matrix diagonalization problem by such approximations. DFT calculations, which are implemented in the Gaussian 09 package with basis set B3LYP/6-31G, are used in the research for optimizing the structure [16], [17], and [18]. We begin our calculation by performing the molecular structure relaxation. After that, we looked at the electronic properties regarding such molecules, including their quantum adsorption parameter, energies, and chemical energy. The next relation was used to calculate the band gap [19], [20], and [21]:

$$E_g = E_{HOMO} - E_{LUMO} \ldots\ldots(1)$$

In which the energies regarding the lowest unoccupied molecular orbital as well as the highest occupied molecular orbital, are denoted by the E_{HOMO} and E_{LUMO}, respectively. We determined the reactivity of CNTs-32-O2, CNTs-32, CNT-32-F2, CNTs-32-CL2, and CNT-32-CO using the DFT calculation and Koopman's theorem. The next parameters have been used to calculate such descriptors, which comprised the ionization potential (IP), chemical hardness (H), electron affinity (EA), and chemical softness (S) [22], [23], [24], and [25]:

$$H = \frac{1}{2}\left[\frac{\partial^2 E}{\partial N^2}\right] \ldots\ldots\ldots\ldots(2)$$

$$S = \frac{1}{2H} = \left[\frac{\partial^2 N}{\partial E^2}\right] \ldots\ldots\ldots(3)$$

Where E, N denoted the total electron energy and the number of the electrons at the constant external potential V(r).

RESULTS AND DISCUSSION GEOMETRIES

For CNTs-CL2, CNT-32-O2, CNTs-CO, and CNTs-F2, the geometry optimization regarding CNTs-32 as well as the gas molecules under investigation is shown in Fig. 1. All of the molecules under study had their equilibrium geometries completely optimized at DFT level of theory with the use of a B3LYP functional in conjunction with the conventional 6-31G basis set in the gaseous phase.

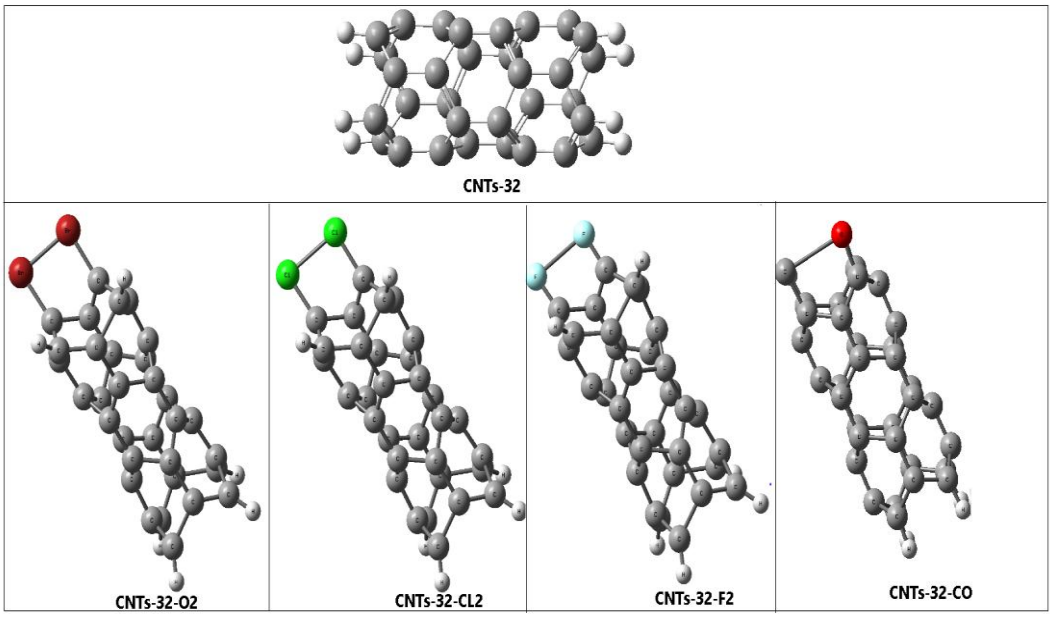

Figure 1. Optimized molecular geometries of CNT_s with the adsorbed O_2, CL_2, F_2, and CO molecules.

In comparison to CNTs-32, Table 1 shows that all total energies have increased, making all structures less reactive and more stable. One crucial characteristic that needs to be investigated is the energy differential between the molecules' energy levels. While low energy gap values indicate that it will be simpler to remove an electron from HOMO orbital to LOMO, which could lead to strong reactivity, large values indicate great electronic stability followed by low reactivity. The findings in Table 1 demonstrate that the energy gap increases when adsorbed O2, F2, CL2, and CO molecules are added to CNTs. The energy levels of CNTs are altered by the presence regarding adsorbed molecules. As a result, CNTs' reactivity and conductivity are decreased. With the maximum energy gap (2.930 eV), this effect was greatest in CNTs-CL2, followed by CNTS-32-F2 (2.881 eV), CNTS-32-O2 (2.822), and CNTs-32-CO (2.770 eV) in that order (see fig.2). The formula used to calculate adsorption energy is [24], [26], [27], [28]:

$$E_{ad} = E_{CNT-32-S} - (E_{CNT-32} + E_S) \ldots\ldots\ldots\ldots (4)$$

Where S represents O2, CL2, F2and CO molecules, $E_{CNT-32-S}$ denotes the CNT-32 adsorption's total energy after adding adsorbed O2, CL2, F2and CO molecules, E_{CNT-32} denotes the molecule's total energy for CNT-32, and E_S denotes the molecule's total energy for O2, CL2, F2and CO molecules. For exploring the possibility of CNT-32

serving as sensors for these compounds, I performed simulations to accurately describe the adsorption behavior of O2, CL2, F2, and CO molecules on a CNT-32, when compared to the other structures, the adsorption energy for CNT-32-O2 is the highest, reaching (-2.5 eV). As a result, the latter's surface experiences high physical adsorption.

Table 1. The electronic properties of CNT_S-32 with the adsorbed O2, F2, Cl_2, and CO molecules.

Structure	HOMO (eV)	LUMO (eV)	Energy gap (eV)	Total energy (a.u)	Adsorption energy (eV)
CNT_S-32	-5.38703	-4.16703	1.220	-982.7819	--
CNT_S-32-O_2	-4.95004	-2.12804	2.822	-1071.5365	-2.5
CNT_S-32-F2	-5.05752	-2.17652	2.881	-1034.6196	-2.8
CNT_S-32-Cl_2	-4.84256	-1.91256	2.930	-1072.5234	-2.7
CNT_S-32-C0	-4.55985	-1.78985	2.770	-1033.4133	-2.9

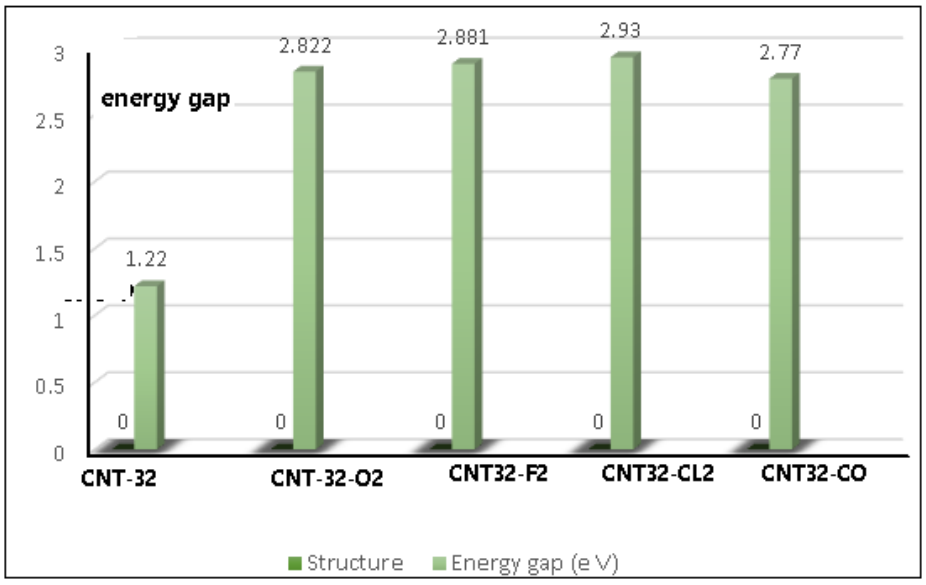

Figure 2. Energy gap of CNT_S-32 with the adsorbed, O2, F2, Cl_2 and CO molecules.

In table 2 showed bond length between C-S1 and C-S2 molecules where S1represents the first atom O1, F1, CL1 and C, while S2 represents the second atom O2, F2, CL2 and O, respectively. In this paper, when comparing the bond length (C-C) before adding the molecules (O_2, F_2, CL_2 and CO) which is equal to(1.34**Å**), while the bond length after adding the aforementioned molecules we notice the expansion of the bond due to the high electronegativity of the atoms. Where the length of the bond reached (1.87 **Å**) for the

($C\text{-}O_2$).

Table 2. Bond lengths (Å) of optimized CNTS-32 and O_2, Cl_2, F_2 and CO here S_1 represents the first atom (O_1, CL_1,F_1 and C_1) and S_2 represents the second atom (O_2, CL_2, F_2 and O_2).

Structure	S_1-C	S_2-C
CNT_S-32	--	--
CNT_S-32-O_2	1.85	1.87

CNT_S-32-F_2	1.465	1.478
CNT_S-32-CL_2	1.542	1.543
CNT_S-32-CO	1.521	1.442

Table 3 shows, the hardness, softness, ionization potential and electron affinity values of CNT32 and CNTs-32-O2, CNT-32-F2, CNTs-32-CL2 and CNT-32-CO separated. These values were computed using equations (2,3), which introduced the hardness and softness features of acid-based chemical processes, based on the energies of the. The values of these parameters represent the charge distribution of the molecule following interaction with adsorption molecules. Additionally, all structures needed more energy to donate or accept an electron in order to be cations or anion because their chemical hardness as well as electron affinity were higher and lower, respectively (see fig. 3). Furthermore, molecules including F_2, O_2, CL_2, and CO formed a strong bond with the CNT-32, which resulted in the structures having a greater electrophilic value.

Table 3. The hardness, softness, ionization and electronic affinity

Structure	Hardness (e V)	Softness (ev)	Ionization (ev)	electronic affinity (ev)
CNT_S-32	0.61	0.81967	5.38703	4.16703
CNT_S-32-O_2	1.411	0.35435	4.95004	2.12804
CNT_S-32-F_2	1.4405	0.34710	5.05752	2.17652
CNT_S-32-CL_2	1.465	0.34129	4.84256	1.91256

CNT_S-32-CO	1.385	0.3610	4.55985	1.78985

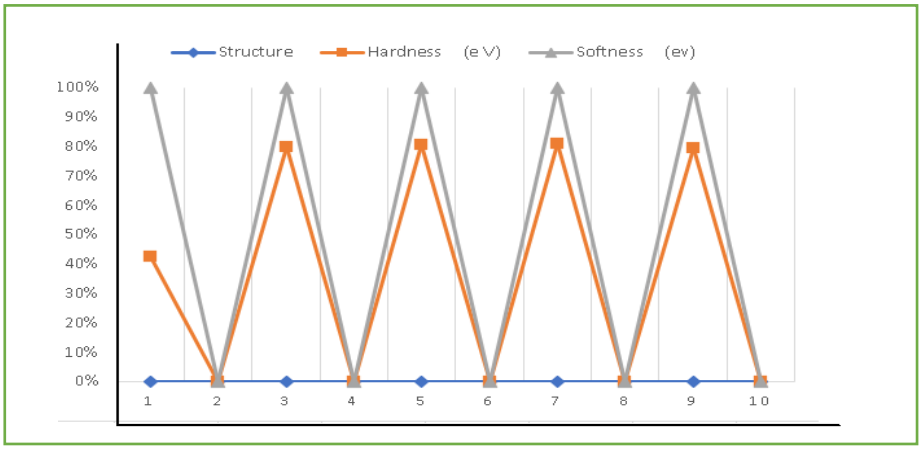

Figure 3. Hardness and Softness of CNT_S-32 with the adsorbed, O2, F2, Cl_2 and CO molecules.

CONCLUSION

Fundamental Finding : DFT calculations are used to study the bonding properties as well as selectivity regarding CNTs-32-O2, CNT32, CNTs-32-CL2, CNT-32-F2, and CNT-32-CO, as well as their adsorption and sensing mechanisms. With the use of B3LYP functional in conjunction with the conventional 6-31G basis set, the electronic structure regarding systems was thoroughly examined. CNTs-CL2 exhibits the largest energy gap (2.930 eV), whilst the CNTs-32-CO exhibits the smallest energy gap (2.770 eV). Furthermore, CNT-32-O2 has the largest adsorption energy, measuring -2.5 eV. **Implication :** The research's findings are helpful in understanding the CNT-32 nanotube as well as in creating extremely sensitive and selective gas detection sensors. **Limitation :** DFT calculations are used to study the bonding properties as well as selectivity regarding CNTs-32-O2, CNT32, CNTs-32-CL2, CNT-32-F2, and CNT-32-CO, as well as their adsorption and sensing mechanisms. **Future Research :** The research's findings are helpful in understanding the CNT-32 nanotube as well as in creating extremely sensitive and selective gas detection sensors.

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