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DFT INVESTIGATION OF CH_2O ADSORPTION ON PRISTINE AND DOPED FULLERENE C_{32}

Abstract: *By using Density Functional Theory (DFT), study the electron properties of the fullerene C_{32} molecules adsorbed with gas (CH_2O). The gas has been placed on the Fullerenes surface in two forms. The first form, the central atom of gas vertically on one of the carbon atom for C_{32} molecule, vertically on one of the phosphorus atom for ($C_{30}P_2$) molecule and vertically on one of the nitrogen atom for ($C_{30}N_2$) molecule. The second form is at the center of the hexagonal ring of carbon atoms of pristine fullerene (C_{32}), the center of the hexagonal ring of ($C_{30}P_2$) molecule and center of the hexagonal ring of ($C_{30}N_2$) molecule using the functional (B3LYP) and the basis set 6-31G (d, p). The results show that, the lowest adsorption energy obtained by gas adsorption with the molecule ($C_{30}P_2$) at the first form and the value of (-0.128 eV) and ($C_{30}N_2$) at the second form and the value of (-0.118 eV) through these result can be considered these cases gas sensors to detect gas (CH_2O). The rest of the cases are also can be used as sensors.*

Key words: *Fullerene, gas adsorption, density functional theory, HOMO and LUMO, sensors.*

Language: *English*

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Introduction

Fullerenes were serendipitously discovered in September 1985 by H. W. Kroto, R. F. Curl and R. E. Smalley During experiments, which involved evaporating graphite by laser irradiation. Their discovery was rewarded with a Nobel prize in chemistry 10-years later in 1996. A new allotropic Fullerene is the third form of carbon along with graphite and diamond. Their distinctive geometric shapes similar to the geodesic dome of the architect R. Buckminster Fuller's led to their being named "Buckminsterfullerene" [1]. Fullerenes or hollow closed carbon cages (C_{2n}) are entirely constructed from the carbon atoms with five- and six-member rings. The number of pentagons is 12 and as the size of fullerene (2n/2–10) increases, the numbers of hexagons would rise [2]. The novel carbon nanostructures discovery has caused many anticipations for their potential effect on gas adsorption, sensing, and storage, by virtue of their large surface /volume ratio. Depending on the valence states the carbon materials demonstrate quite different adsorption properties. In the last years, nanotubes have attracted great interest in the sensor industry [3].

2. COMPUTATIONAL DETAILS OF DFT

In this work, DFT calculations were performed using Gaussian 09 package [4]. This software package is using the standard and modern quantum mechanics basics The functional B3LYP/6-31G(d,p) basis set is used for the full geometry optimizations of the adsorption influence of CH_2O molecules on C_{32} and doped $C_{30}P_2$, $C_{30}N_2$ [5]. The functional B3LYP/6-31G(d,p) is a commonly used level of theory for

nanotube structures [6-7]. The chemical potential or Fermi energy (E_F) of the complexes was obtained, as given below:

$$E_F = E_{HOMO} + E_{LUMO} / 2 \quad (1)$$

Where E_{HOMO} is the energy of the highest occupied molecular orbital and E_{LUMO} is the energy of the lowest unoccupied molecular orbital. The energy gap in energy levels (E_g) of a system is acquainted as:

$$E_g = E_{LUMO} - E_{HOMO}. \quad (2)$$

The adsorption energy (E_{ads}) was calculated using the following approximate expression:

$$E_{ads} = E_{(COMPLEX)} - (E_{(molecule)} + E_{(gas)}) \quad (3)$$

Where $E_{(COMPLEX)}$ is the total energy of the molecule with adsorption with gas, $E_{(molecule)}$ is the total energy of the studied molecule without adsorbed, and $E_{(gas)}$ is the total energy of the gas molecule [8,9].

After geometry optimization, the adsorption energy (E_{ads}) and electronic properties of the studied molecules like HOMO, LUMO, Total energy (E_{Tot}), Energy gap (E_g), Electron Affinity (EA), Ionization Potential (IP) and Fermi Energy (E_F) were found as shown in Table 1.

Table 1: Structural and electronic properties of the studied complexes.

Property (eV)	C_{32}		$C_{30}P_2$		$C_{30}N_2$	
	a	b	c	d	e	f
E_{Tot}	-36277.738	-36277.776	-52782.305	-52782.320	-37184.169	-37184.144
E_{ads}	-0.275	-0.313	-0.128	-0.142	-0.144	-0.118
E_g	1.522	1.528	1.616	1.618	1.580	1.568
IP (= $-E_{HOMO}$)	5.144	5.217	5.340	5.384	5.311	5.219
EA (= $-E_{LUMO}$)	3.622	3.688	3.724	3.765	3.731	3.650
E_F	-4.383	-4.452	-4.532	-4.574	-4.521	-4.435

3. RESULTS AND DISCUSSION

The adsorption behavior of CH_2O gas molecule on the surface of pristine fullerene C_{32} and heterofullerenes $C_{30}P_2$, $C_{30}N_2$ are examined. Initially, each gas molecule has been placed on the Fullerenes surface in two forms. The first form, the central atom of gas is close to one of carbon, phosphorus, and nitrogen atoms of C_{32}, $C_{30}P_2$ and $C_{30}N_2$ respectively, and in the second form, the gas molecule is located on the top of the hexagonal ring of C_{32}, $C_{30}P_2$, and $C_{30}N_2$. It was found that the C_{32}, $C_{30}P_2$, and $C_{30}N_2$ distances for CH_2O absorption are in the range of (3.39-4.6 Å), the bond length of the atom between the carbon atom and the oxygen atom is (1.20 Å) of the gas (see Figure 1).

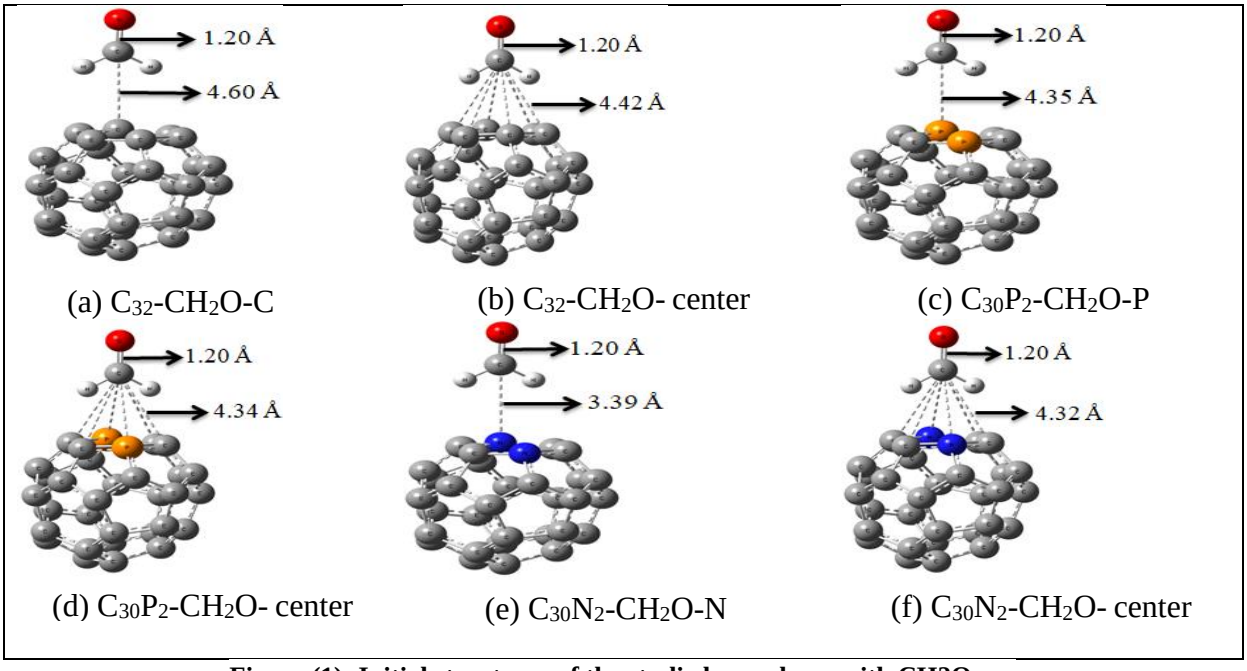

Figure (1): Initial structures of the studied complexes with CH2O gas

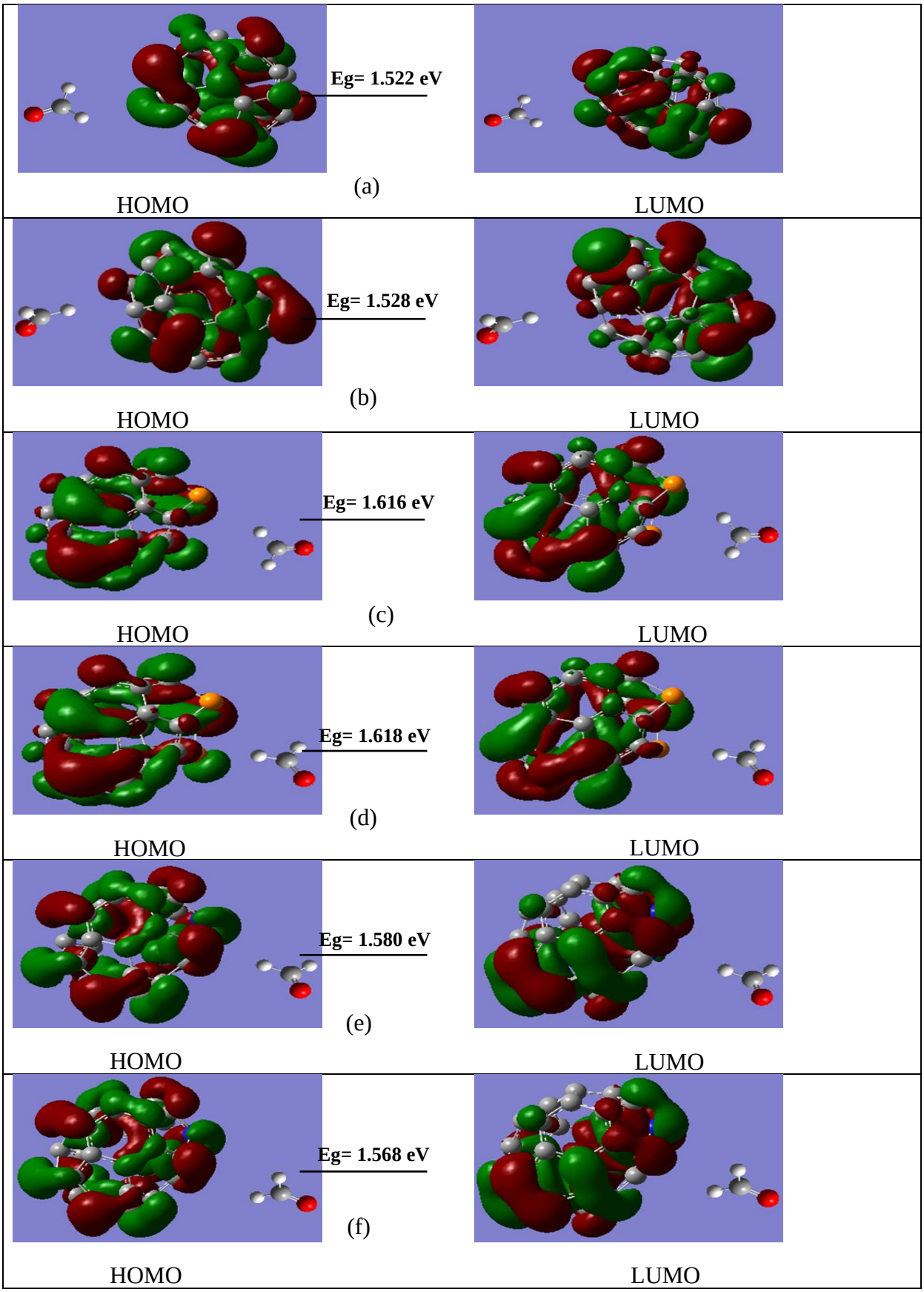

Figure 2: Shows the DFT calculation of HOMO and LUMO shapes for studied CH_2O adsorption molecules.

Fig. 2 shows that in HOMO and LUMO the lobes are concentrated on almost all the atoms and are not concentrated on the gas in all cases because they are adsorbed with the molecule. In the molecules $C_{30}P_2$ and $C_{30}N_2$ the lobes are concentrated around the phosphorus and nitrogen atoms and the neighboring atoms, with no concentration of gas. The adsorption energy of $C_{30}P_2$, at the site (c), is (-0.128 eV) and the adsorption energy of $C_{30}N_2$ at the site (f), is (-0.118 eV). For this reason, $C_{30}P_2$ at the site (c) and $C_{30}N_2$ at the site (f) can be used as a sensor to detect CH_2O, gas. Also, the adsorption energy that has been obtained for all cases can be used as a sensor to detect this gas.

4. CONCLUSIONS

We explore the adsorption of CH_2O, on the surface of fullerene C_{32} and doped fullerenes by DFT calculation at B3LYP/6-31G(d,p) level of theory. In general, the adsorption energies in the results indicate that C_{32} and doped fullerenes are weak physisorption, in all sites and can be used to detect CH_2O. For $C_{30}P_2$ at the site (c) and $C_{30}N_2$ at the site (f) can be used as a sensor to detect CH_2O since the adsorption-desorption equilibrium of CH_2O on $C_{30}P_2$ and $C_{30}N_2$ at these sites is easily built gas. The adsorption energy of $C_{30}P_2$, at the site (c), is (-0.128 eV) and the adsorption energy $C_{30}N_2$ at the site (f) is (-0.118 eV). Finally, the results of calculations show that these adsorption configurations are suitable as sensors of CH_2O.

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