Int.J.Nano Dim. 2(4): 281-284, Spring 2012
ISSN: 2008-8868

Contents list available at **IJND**

International Journal of Nano Dimension

Journal homepage: *www.IJND.ir*

Short Communication

Preparation and investigation of the adsorption effects of CO_2 on the hardness of the SWCNT (8,0) by gap HOMO-LUMO

Kh. Tavakoli[1,*]
M. Keshavarz[2]
A. kazemi[1]

[1]ChemistryDepartment,Shahrekord Branch, Islamic Azad University, Shahrekord, Iran.
[2] Chemistry Department, shahreza Branch, Islamic Azad University, shahreza, Isfahan, Iran.

Received: 09 May 2011
Accepted: 15 July 2011

* Corresponding author:
Khadijeh Tavakoli
[1]Chemistry Department, Islamic Azad University-, Shahrekord Branch, Shahrekord, Iran.
Tel +98 9194704299
Fax +98 3213213103
Email tavakoli.khadijeh@yahoo.com

ABSTRACT

In this study the hardness SWCT was calculated with B3LYP,HF method and 3-21G,6-31G,6-311G basis set .Then it was investigated with the best method(B3LYP) and basis set(6-31G) to study the adsorption effects CO_2 on the hardness of SWCNT with gap HOMO-LUMO in two shape: Horizontal, Vertical and Top-Center-Bridge and We also provide the effects of CO_2 adsorption on the electronic properties(DOS) of the CNTs. The soft wares which were used in this study were Gaussian 03w; Gauss view 5.0w and Nano tub modeler. The Purpose of this study is to compare the effects of the basis set&CO_2 adsorption on the hardness of SWCNT (8, 0) in gases phase.

Keywords: *Hardness; SWCNT; DFT; HOMO-LUMO,DOS.*

INTRODUCTION

The first report by Iijimal[1] was on the multiwall form,coaxial carbon cylinder with a few tens of nanometers in outer diameter. Two years later single walled nanotubes were reported [2,3].Recent studies have shown that the physical properties of single-wall carbon nanotubes(SWCNT)could be modified by adsorption of the foreign atoms or molecules[4,6].Gas adsorption on carbon nanotubes is an important issue for both the fundamental research and technical applications of nanotubes. Selective reduction of nitrogen monoxide (NO) in oxidizing atmosphere has recently received much attention because it has a potential as a practical measure to remove NO_X emitted from diesel lean burn engines [7]. Recently, CO_2 adsorption on SWCNTs has received attention [8-9] because the understanding of the adsorption of CO_2on SWCNTs is relevant to the potential use of SWCNTs in the separation of CO_2 which is both a respiratory gas and the most important green house gas. Zhao et al. studied the adsorption energies of CO_2 and other small gas molecules on SWCNTs using the local density approximation-density functional theory (LDA-DFT) [10].

COMPUTATIONAL METUODS

The calculations have been carried by using the Gaussian 0.3 W suite of programs. The density functional method with the B3LYP functional and the 6-31G basis set was used for all the calculations. In the first step, (8,0) Zigzag carbon nanotube (CNT) with length 10 ºA has been selected and the ends of nanotube are saturated by hydrogen atoms. The hydrogenated (8,0) carbon nanotube have 84 atoms and the structure have the diameter of ~1/4 ºA .various orientations of CO2 surface the (8,0) carbon nanotube are considered. The adsorption energy of CO_2 surface of the CNT for all the geometries was calculated as follows: Eads = ECNT/CO_2 – [ECNT +ECO_2].

RESULTS AND DISCUSSION

There are many experimental and theoretical results available on the structural parameters of CO_2.

In the present study, the structural parameters of CNT obtained at the DFT (B3LYP, B1LYP), HF /6-31G level of calculation are given in Table1.we limited our analysis to interaction of CO_2 with the nanotubes (8,0) outer walls. Considering each site and configuration, we ended up with nine different approaches of CO_2 to the CNT-CO_2 walls .for each of these cases we investigated the CNT-CO_2 Single-Point Energy(SPE) at the B3LYP/6-31G method. The B3LYP/6-31G methods are plotted in graph1and HOMO-LUMO shapes showed in Figure 1 and 2. All the results are clearly summarized in Table1 and 2.

Electronic properties

To better understand the nature of interaction between the CO_2 and the CNTs, we studied the influence of CO_2 adsorption on the electronic properties of the CNTs. As evident from Figure 3, the calculated band gap of the CO_2 adsorbed (8,0) CNTs is -20.0 ev. The total densities of states (DOS) of this tube did not show changes due to CO_2 adsorption in the gap regions of the TDOS plots. The effects of the CO_2 on adsorption energies in the CNTs relate to their electronic structure. When the CO_2 is adsorbed on the CNTs, the interaction of between them being very weak, the electronic properties of these tubes are not changed obviously. This trend is agreement with the CO_2 adsorption on the CNTs.

Table.1. Energy and hardness single-wall carbon Nanotubes

Species	Method	Basis set	E_{SWNT} (Hartree)	HOMO	LUMO	η
SWCNT(8,0)	HF	3-21G	-2418.85043155	-0.18604	-0.06081	0.062615
	B1LYP	6-31G	-2446.44260251	-0.23009	-0.11256	0.058765
	B3LYP	6-31G	-2447.68357518	-0.22857	-0.12282	0.052875
		6-311G	-2448.1326507	-0.23740	-0.12477	0.11263
		6-31G*	-2448.27698191	-0.22504	-0.12037	0.052335

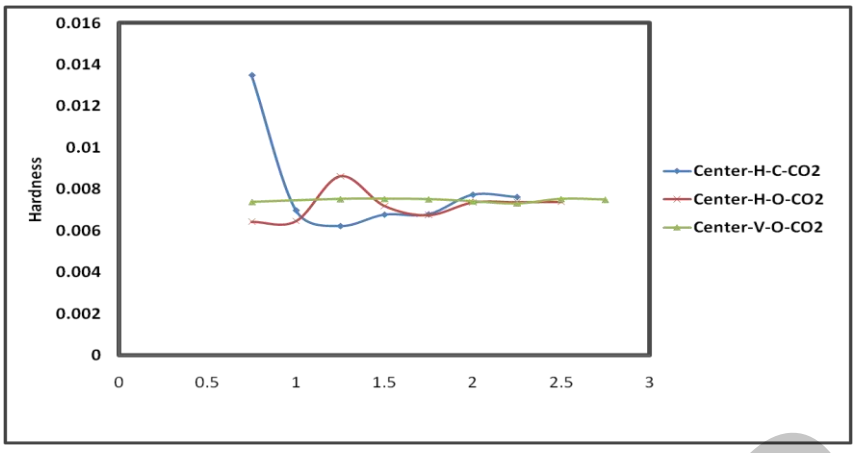

Fig.1. Change of Hardness of Nanotube due to adsorption of carbon dioxide at Center state.

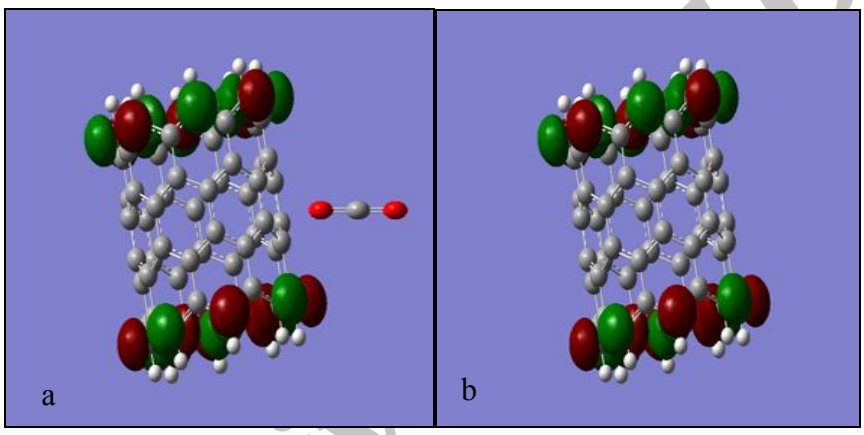

Fig.2. HOMO-LUMO Gap nanotube (a), CNT-CO_2 (b)

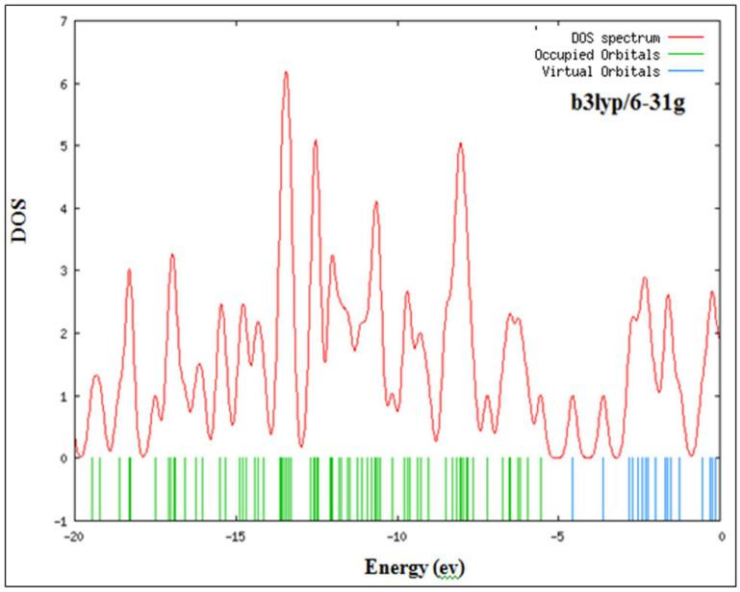

Fig. 3. The total densities of states (DOS) for the CO_2 adsorbed on the (8,0) CNTs in most stable configuration.

Table.2. Change of Hardness of Nanotube due to adsorption of carbon dioxide at TOP state

R(CO_2-CNT)/ $^{\circ}$A	H-C	V-O
2.25	0.00752	**0.00752**
2.5	0.00707	**0.007535**
2.75	0.007525	**0.007535**
3.00	0.00755	**0.007405**
3.25	0.00755	**0.007545**
3.5	0.00755	**0.007545**
3.35	0.00755	**0.0075**
4.00	0.00754	**0.0075**
4.25	0.007535	**0.00752**

CONCLUSION

In this study we investigated the adsorption and hardness of co on swcnt (8,0) with two orientations of c-down and o-down.

The following results were obtained in the study of biatomic gas (CO_2) adsorption on surface SWCNT (8,0) : Adsorption occurred on the outside and inside of the nanotube. The adsorption energies obtained show that, CO_2 molecule is more stable than the other gases. Finally We found that adsorption of biatomic gases molecules on SWCNT is accompanied, so H_2, CO_2 molecules are weakly adsorbed on SWCNT (8,0). The high distance hardness decries CNT.

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