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NBO analysis and theoretical thermodynamic study of (5,5) & (6,6) armchair carbon nanotubes via DFT method

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ABSTRACT: In the present work, the structural and electronic properties, and conductivity of (5,5) and (6,6) Single Walled Carbon Nanotubes in the ground state have done by using the Hartree-Fock and density functional theory DFT-B3LYP/6-31G* level. Delocalization of charge density between the bonding or lone pair and antibonding orbitals calculated by NBO (natural bond orbital) analysis. These methods are used as a tool to determine structural characterization CNTs in the gas phase. The total electronic energy, dipole moment, natural atomic orbital energies, charge density, density of state (DOS), highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO) energies, HOMO-LUMO energy bond gaps, the global index includes hardness (η), electronegativity (χ), electrophilicity index (w), chemical softness (S) and electronic chemical potential (μ) were calculated. We have reported our investigation on the conductivity and electronic structures of pure (5,5) and (6,6) SWCNTs. The calculated HOMO-LUMO energy bond gap show that charge density transfer occurs within the molecule and the results indicate that the conductivity of the CNTs, and also the semi conductivity could be justified.

Keywords: *Carbon nanotubes; Conductivity; DFT Calculation; Energy bond gap; NBO analysis*

INTRODUCTION

The carbon nanotubes are more considerable nanostructures with a large variety of potential applications in the fields of environmental technologies, as electrochemical systems and sensors in nanoelectronics. After the discovery of carbon nanotubes (CNTs) by (Iijima, 1991), numerous works have been devoted to study the mechanical and electrical properties and applications of carbon nanotubes (CNTs) (Sinha and Yeow, 2005). CNTs are a new allotrope of carbon originated from fullerene family (Daniel, *et al.*, 2007). However, based on nanotubes properties exhibiting absorption or storaging behavior depending upon the tubular diameter and length, and are influenced by atomic arrangement (chirality) (Wei, *et al.*, 2001, Maruccio, *et al.*, 2004). Carbon nanotubes have been recently studied due to their importance as building blocks in nanotechnology (Buldum, *et al.*, 2002, Ulbricht, *et. al.*, 2002), and also They have used as molecular containers with applications such as hydrogen fuel cells (Fischer, 2000, Meunier, *et al.*, 2002), nanoelectronic devices, transistors, and chemical and electrochemical sensors, gas sensors, and so many

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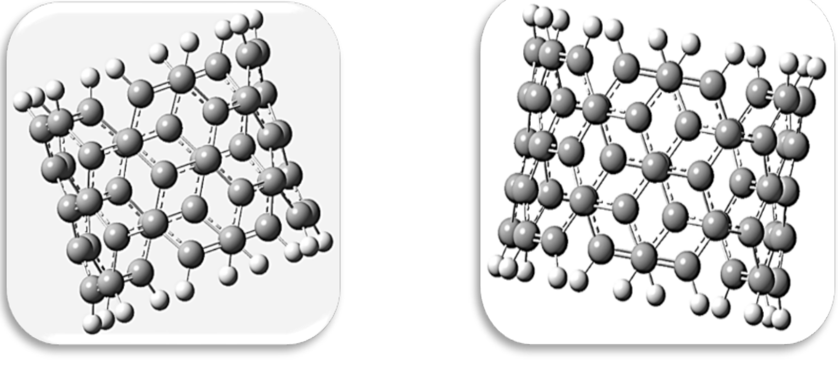
other applications (Dresselhaus, *et al.*, 1996, Saito, *et al.*, 2001, Zhao, *et al.*, 2000, Meyyappan, 2004). CNT can be classified into single-walled nanotubes (SWNTs) and multi-walled nanotubes (MWNTs) according to the number of layers of the rolled graphite (Foley, 2005). They have three conformations: armchair (n, n), zigzag (n, 0) and chiral (n, m) these conformations have individual properties (Gojman, *et al.*, 2004). The most interesting attention in the SWNTs is that their electronic structures depend on the chirality and diameter. SWNTs are (1) metals when n = m, (2) narrow gap semimetals when n-m is a multiple of three, and (3) moderate-gap semiconductors otherwise, where (n, m) is the chiral index (Hamada, *et al.*, 1992, Lai, *et al.*, 2008). Single-walled nanotubes (SWNTs) have been contemplated as the most important candidate for nanodevice applications because of their one-dimensional electronic structure, biocompatibility, property of conducting electrical current and reversible response to biological reagents hence they formed bonding to biological structures such as carbohydrates and nucleotides and polymers (Ramanathan, *et al.*, 2005). Previous studies indicated that CNTs are very significant structure, and applications of Single-walled nanotubes (SWNTs) are extensively spread out from nanobiotechnology to nano-matematic, e.g., (Jin, *et al.*, 2006, Harris, 1999). However based on CNTs properties revealing chemical and electrochemical sensors, biosensors, transistors and the most other applications, therefore, considerable attempts have been raised to experimentally synthesis or theoretically investigation the stable structure of SWCNTs (Baughman, *et al.*, 1999, Loiseau, *et al.*, 1998). In this work, the chemical properties, electrical conductivity and reactivity of (5,5) and (6,6) armchair SWCNTs is investigated with using Hartree-Fock approximation, Density Functional Theory (DFT)/B3LYP calculations and NBO interpretation on (5,5) and (6,6) SWCNTs are performed, and also, the effect of various basis set upon total energy of structure have been studied.

COMPUTATIONAL DETAILS

In this study, representative model of SWCNTs was optimized using the Gaussian 03 package of program (Frisch, *et al.*, 2004). The (5,5) CNT consists 50 C atoms and the two ends of the tube are capped by 20 H atoms, also the diameter of the nanotube is 6.71 Å, and the length of the nanotube is 4.88 Å and the (6,6) CNT consists 60 C atoms and the two ends of the tube are capped by 24 H atoms, also the diameter of the nanotube is 8.32 Å, and the length of the nanotube is 4.88 Å (see Fig. 1). Density Functional Theory method and Hartree-Fock approximation are used to investigate the structural and electronic properties of the tubular systems. The calculations were performed with the HF and DFT/B3LYP functional and 6-31G* level of theory. An NBO (Natural Bond Orbital) analysis was performed using the HF and DFT/B3LYP methods to determination of electron density delocalization between the bonding or lone pair orbital Lewis type and antibonding orbital non-Lewis calculated by the NBO 5.G program via the PC-GAMESS interface (Becke, 1992, Glendening, *et al.*, 2004, Reed, *et al.*, 1988).



(5,5) CNT (6,6) CNT

Fig. 1. Atomic structures of armchair (5,5) and (6,6) Single Walled Carbon Nanotubes.

RESULTS AND DISCUSSION

The thermodynamic parameters (ΔG, ΔS and ΔH) between the most stable (5,5) and (6,6) SWCNTs and the relative energy difference values (ΔE_0) as calculated at the B3LYP/6-31G* and HF/6-31G* levels of theory, are given in Table 1. The results disappear that the (6,6) armchair SWCNT is more stable than the (5,5) armchair SWCNT. The electronic structures depend on the chirality and diameter in SWNTs is more significant to explain the stability and reactivity of Single Walled Carbon Nanotubes. The values of calculated Gibbs free energy difference (ΔGeq−ax) of compounds (5,5) and (6,6) SWCNTs by the DFT/B3LYP and the HF methods show that the (6,6) armchair SWCNTs with the diameter of 8.32 Å is more stable than the (5,5) armchair SWCNT with the diameter of 6.71 Å it could establish the role of diameter in SWNTs to determination of conductivity and chemical activity of CNTs.

The hybrid DFT (hybrid-density functional theory) and ab initio molecular orbital calculations were carried out using the HF/(6-31G*) and B3LYP/(6-31G*) levels of theory to investigation of the electronic structural behaviors of pure armchair (5,5) and (6,6) Single Walled Carbon Nanotubes. The DFT methods have been useful in rationalizing concepts such as selectivity of chemical structures based on reactivity indices of molecules. The global index includes hardness (η), electrophilicity index (w), electronegativity (χ) and softness (S) (Sen and Jorgensen, 1987, Gomez and Martinez-Magadan, 2005, Chattara and Poddar, 1999). For an N-electron system with a total energy (E) and total external potential ν(r), the maximum amount of electronic charge index (ΔN_{max}), amount of hardness (η), softness (S) and electronegativity (χ) of the equilibrium state at (T) temperature are calculated as the following equations:

$$\chi = -\left(\frac{\partial E}{\partial N}\right)_{\nu(r),T} = -\mu \tag{1}$$

$$\eta = \frac{1}{2}\left(\frac{\partial^2 E}{\partial N^2}\right)_{\nu(r),T} = \frac{1}{2}\left(\frac{\partial \mu}{\partial N}\right)_{\nu(r),T} \tag{2}$$

$$S = \frac{1}{2\eta} = \left(\frac{\partial N}{\partial \mu}\right)_{\nu(r),T} \tag{3}$$

Where (μ) is the electronic chemical potential, Furthermore, an electrophilicity index (w) (Pearson, *et. al.*, 1999) has recently defined as:

$$w = \left(\frac{\mu^2}{2\eta}\right) \tag{4}$$

Pauling explained the meaning of electronegativity as the ability of an atom in molecule to attract electrons and electrophilicity index (w) was suggested as a measure of the electrophilic ability of molecules. The Milliken charge densities of tube-molecules were estimated by NBO calculations. The NBO result shows the partial charges on the whole of carbon atoms. The value of dipole moment was calculated by using of DFT/B3LYP method. It is considerable that dipole moment is a measure of asymmetry in charge distribution of molecules.

Chemical potential (μ) of molecule is calculated using Koopmans theorem (Zevallos and Toro-Labbe, 2003, Chattaraj and Poddar, 1999), E_{HOMO} plus E_{LUMO} as follows:

$$\mu = \frac{(E_{HOMO} + E_{LUMO})}{2} = -\chi \tag{5}$$

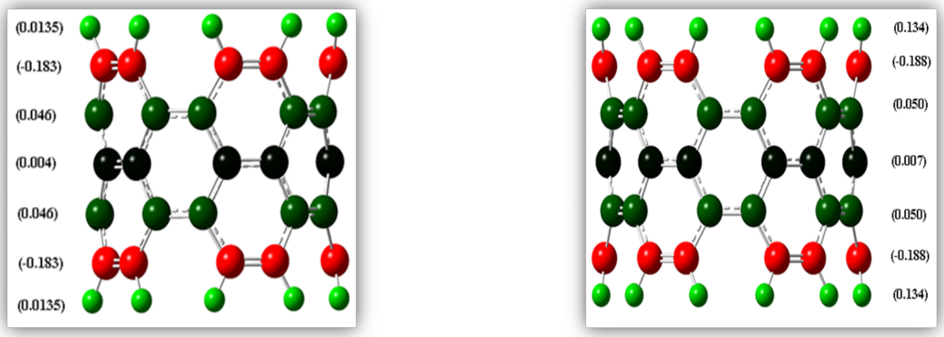
This definition was driven from (Eq. 1).

Table 1: The calculated B3LYP/6-31G*, HF/6-31G* relative energy difference values (ΔE_0) and thermodynamic parameters [ΔH, ΔG (in hartree) and ΔS (in cal $mol^{-1}K^{-1}$)] differences at 25ºC and 1 atm pressure for (5,5) and (6,6) SWCNTs.

	B3LYP/6-31G*//B3LYP/6-31G*				HF/6-31G*//HF/6-31G*			
Compounds	G	S	H	E_0	G	S	H	E_0
(5,5) CNT	-1916.843	170.63	-1916.762	-1916.792	-1904.469	161.76	-1904.392	-1904.419
(6,6) CNT	-2300.307	195.83	-2300.214	-2300.250	-2285.465	182.21	-2285.379	-2285.411
	ΔG^a	ΔS^a	ΔH^a	$\Delta E_0{}^a$	ΔG^a	ΔS^a	ΔH^a	$\Delta E_0{}^a$
	383.464	-25.195	383.452	383.458	380.996	-20.452	380.986	380.992

Table 2: Comparison of Dipole Moments (Debye), chemical hardness (in hartree), chemical softness (S) (in hartree-1), electronic chemical potential (μ) (in hartree), the Muliken electronegativity (χ) (in hartree), electrophilicity index (w) (in hartree), the maximum amount of electronic charge index (ΔN_{max}) (in hartree), E_{HOMO}-E_{LUMO} energy gaps (in hartree) and Total Electronic Energy (in hartree) calculated for (5,5) and (6,6) SWCNTs by using B3LYP/6-31G*method.

Compounds	Dipole Moment	η	S	μ = - χ	w	ΔN_{MAX}	E_{HOMO}	E_{LUMO}	Band Gap	Total Energy (SCF Done)
(5,5) CNT	0.00	0.041	0.020	-0.121	0.180	2.951	-0.161	-0.080	0.081	-1917.318
(6,6) CNT	0.00	0.035	0.017	-0.122	0.214	3.486	-0.157	-0.088	0.070	-2300.883



(5,5) CNT (6,6) CNT

Fig. 2. The Mulliken atomic charges of armchair (5,5) & (6,6) Single Walled Carbon Nanotubes.

Chemical hardness (η) (Prystupa, *et. al.*, 1994) is calculated as:

$$\eta = \frac{(E_{LUMO} + E_{HOMO})}{2} \qquad (6)$$

$$\Delta N_{max} = \frac{-\mu}{\eta} \qquad (7)$$

The electronic chemical potential (μ), the global index includes electronegativity (χ), chemical hardness (η), softness (S), electrophilicity index (w), the maximum amount of electronic charge index (ΔN_{max}) and dipole moment were calculated by using DFT/B3LYP method are listed in Table 2.

The Mulliken atomic charges distribution of armchair (5,5) and (6,6) Single Walled Carbon Nanotubes is shown in Fig. 2 as colored carbon and hydrogen atoms.

Considering HOMO-LUMO energy bond gap and chemical hardness shows that a soft molecule has small HOMO-LUMO energy gap and a hard molecule has a large HOMO-LUMO energy gap (see Table 2). On the other hand, the stability and reactivity of a molecule relates to energy bond gaps, which means the mol-

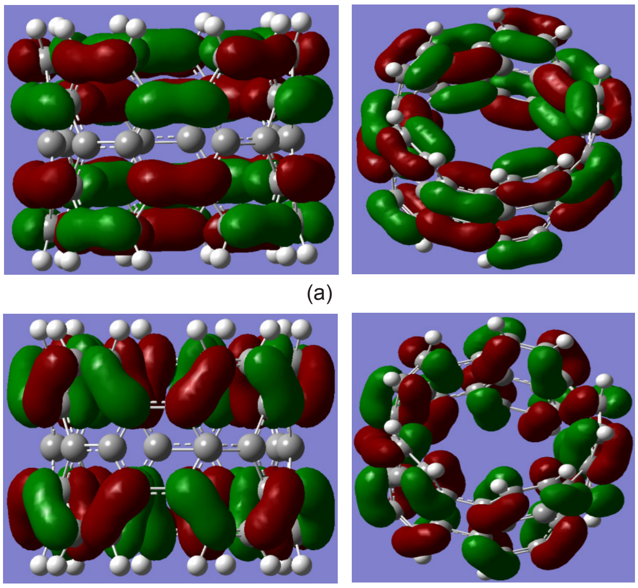


Fig. 3. The HOMO and LUMO frontier molecular orbitals of armchair (5,5) SWCNT from the different sides.

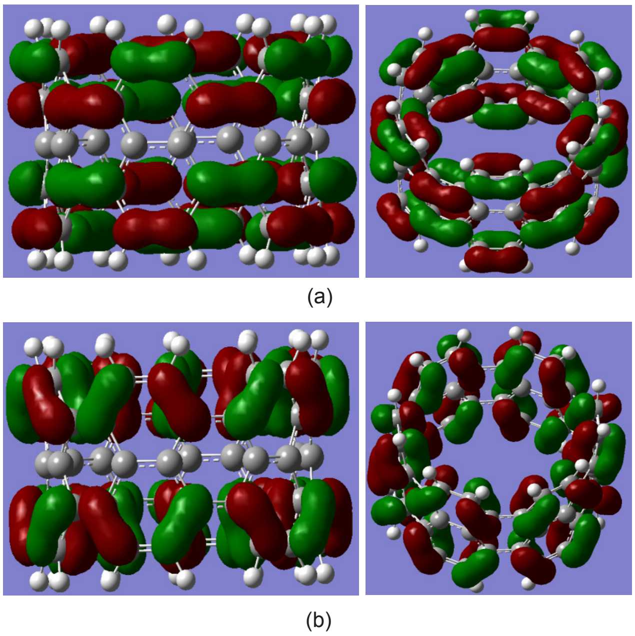


Fig. 4. The HOMO and LUMO frontier molecular orbitals of armchair (6,6) SWCNT from the different sides.

ecule with least HOMO-LUMO energy gap is more stable because of high electron delocalization between HOMO & LUMO frontier orbitals (Figs. 3, 4). The stabilization orbital interactions should increase as the donor orbital energy increases and the acceptor orbital energy decreases. Moreover, the electron delocalization in the CNTs could be justified by variation of Orbital Occupancies. The decrease of the bonding orbital occupancies and the increase of the anti-bonding orbital occupancies in the SWCNTs could be explained by the decrease of energy differences between donor and acceptor orbitals for the SWCNTs that cause to electron distribution in these compounds. Table 2 shows the calculated values of HOMO-LUMO energy gap and total electronic energy of armchair (5,5) and (6,6) SWCNTs. As DFT-based methods provide useful information to describe the structural properties of CNTs, moreover, the DFT results are comparable with experimental values.

The obtained results shows that with increasing basis set, precision and accuracy of the calculated total electronic energy (E_{el}) value and the other structural parameters is increased. Also, The calculated E_{el} by B3LYP/6-31G* level of theory is slightly lower than HF method (see Table 2). The total densities of states (DOS) is obtained using HF and B3LYP methods with the best used basis set (6-31G*) for armchair (5,5) and (6,6) Single Walled Carbon Nanotubes in most stable configuration and are revealed at Fig. 5.

Organic compounds including conjugated π electrons by the large values of polarisability were investigated by means of spectroscopy (Pearson, *et al.*, 1978). The intermolecular charge density transfer from the donor to acceptor group in conjugated π electrons systems through single-double bonds conjugated can persuade variations in both the molecular polarisability and dipole moment. The experimental result that indicates large Raman and IR intensities for these compounds were recorded and are comparable with theoretical calculations (Sundaraganesan, *et al.*, 2009). The wave function analysis shows that the electron charge transfer carries out from the HOMO energy (ground state) to LUMO energy (first exited state). The NBO result

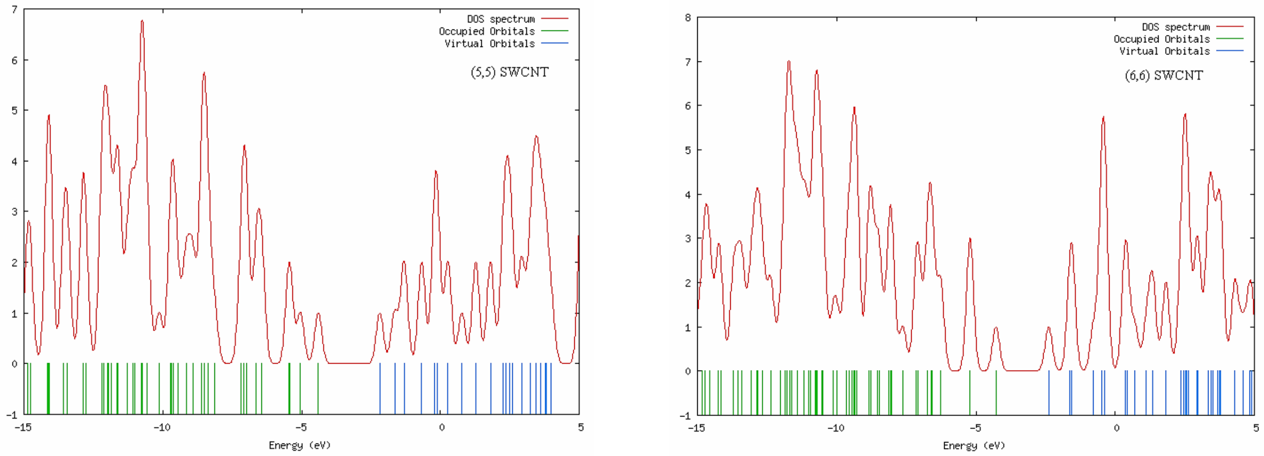


Fig. 5. The total densities of states (DOS) is calculated using HF/6-31G* and B3LYP/6-31G* levels of theory for armchair (5,5) & (6,6) Single Walled Carbon Nanotubes in most stable configuration.

reveals that the energy gap appears the measure of chemical activity, stability and electrical conductivity of CNT compounds. Considering the small HOMO−LUMO energy bond gap and the measure of chemical hardness means a soft compound and it related to molecular property of conducting electrical current. The results clearly indicated that, the increase in global hardness and energy gap reveal the increasing of stability and decrease reactivity of the SWCNTs.

CONCLUSIONS

The ab initio molecular orbital calculation and hybrid DFT (hybrid-density functional theory) were carried out using the HF/6-31G* and B3LYP/6-31G* levels of theory. Comparison of Hartree-Fock and DFT/B3LYP calculated results indicate that the DFT method is superior than the HF approach to investigation of chemical and physical properties. In order to determinate conductivity and chemical activity of CNTs, the electronic chemical potential (μ) chemical hardness (η), chemical softness (S), and the E_{HOMO}-E_{LUMO} have been calculated by NBO analysis. To draw a conclusion, the obtained result shows that, the charge transfer occurs within the SWCNTs that give rise to the conductivity of carbon nanotubes. Considerable used method not only shows the way to characterization of CNTs, moreover, it will be more effective in fundamental investigations in chemistry and biochemistry sciences.

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