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NMR Shielding Tensors and Thermodynamic Investigation of TWCNTs including BN Doping: A model for H_2 storage

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ABSTRACT

B3LYP/6-31G/6-31G/6-31G*/6-311G* density functional theory (DFT) calculations have performed for the structure and stability of three wall carbon nano tubes (TWCNTs). In this work, it was calculated the geometrical structure, and stability to predict NMR and thermodynamics parameters. A mixing of SWBNNTs @ DWCNTs has been modeled and calculated for the suitable structures to storage the H2 molecules. We have found these kinds of nano-structures are useful for maximum storages of H2 molecule compare to other SWCNTs.

Key words: Storages of H2 molecule, Density functional theory (DFT), Ab-initio calculation, Thermodynamic parameters.

INTRODUCTION

Although much study has been done for nanotube carbon phenomenon, there are a few studies for MWCNTs such as TWCNTs[1-10]. The carbon nanotube (CNT) is a representative nano-material. CNT is a cylindrically shaped carbon material with a nano-metric-level diameter[3-12].

Its structure, which is in the form of a hexagonal mesh, resembles a graphite sheet and it carries a carbon atom located on the vertex of each mesh. The sheet has rolled and its two edges have connected seamlessly[5-15].

Although it is a commonplace material using in pencil leads, its unique structure causes it to present characteristics that had not found with any other materials. CNT can be classified into single-wall CNT, double-wall CNT and multi-wall CNT according to the number of layers of the rolled graphite[10-20]

The type attracting most attention is the single-wall CNT, which has a diameter deserving the name of “nanotube” of 0.4 to 2 nanometers. The length is usually in the order of microns, but single-wall CNT with a length in the order of centimeters has recently released[19-25].

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The length is usually in the order of microns, but single-wall CNT with a length about centimeters have recently released. The extremities of the CNT have usually closed with lids of the graphite sheet[21-30].

The lids consist of hexagonal crystalline structures (six-membered ring structures) and a total of six pentagonal structures (five-membered ring structures) placed here and there in the hexagonal structure[22-35]. The first report by Iijima was on the multiwall form, coaxial carbon cylinders with a few tens of nanometers in outer diameter. Two years later, up to now, single walled nanotubes were reported in various works[5-20]. SWCNTs have considered as the leading candidate for nano-device applications because of their one-dimensional electronic bond structure, molecular size, and biocompatibility, controllable property of conducting electrical current and reversible response to biological reagents hence SWCNTs make possible bonding to polymers and biological systems such as DNA and carbohydrates[30-35].

Boron nitride nanotube (BNNTs) have attracted much interests due to their large gap semi conducting character[20-55].Boron nitride (BN) is a structural existing in cubic (diamond-like), hexagonal (graphite-like), turbo static, and amorphous forms .these compounds have been produced by a variety of methods, such as arc melting[50-59], high temperature chemical reaction[44-59], carbon nanotube templates[50-66], and laser ablating[52-69] The most attention has been focused on the development of new methods for the production of nanotube and inorganic fullerene of other materials.

In addition**,** theoretical calculations have been described the possible existence of small BN clusters[57-77].

Theoretical studies have been performed for BN doped in CNTs which it has been found that a structure built from squares and hexagons is more stable than those built from pentagons and hexagons. This is because in the second case less stable B-B and N-N bonds are formed[65-90].

The most stable TWCNTs structure is built from CNTs doping with BN[70-104]. In this work, we focused on TWCNTs and TWC (BN) NTs nano-con. Our aim was to obtain the global minimum energy structure. For this structure, we use the hybrid B3LYP exchange-correlation functional within density functional theory. Primary, structure optimization calculated and then Nuclear Magnetic Resonance (NMR) parameters by density Functional Theory (DFT) method calculated on the optimized structure. Isotropic chemical shielding, anisotropic chemical shielding parameters at all of the atoms nuclei are presented in Table 1. And also, Thermodynamic Properties have been considered in Table 2

We have found that these kinds of Nano-tubes are useful for H2 Storage. In material sciences Boron nitride, which appears in a manifold of crystalline modifications, has been an extremely practical material with hexagonal and cubic boron nitride as most outstanding materials (for doping). The BN cluster is a polar molecule and BN doped in nanotubes have an inert chemical structure. We can see that there is a negative charge at nitrogen atom and a positive charge at boron atom, so we can use an electrophilic or nucleophilic reagent as a solution for BN clusters.

BN nanotubes are very suitable for composite materials because these structures have a higher temperature resistance to oxidation than the carbon nanotubes. All the BN nanotubes are semiconductors. The BN doped in nanotubes have the band gaps which can be greater than 2 eV for most tubes also we know that the smallest carbon nanotubes are semiconductor and these structures obtain the properties of graphite when the diameter of these structures increases but BN nanotubes are semiconductors without attention to the diameter. On the basis of the similarities in characteristics between carbon and BN-based (BN=boron nitride) substances, BN-based nanotubes can be stable and therefore their electronic structure can be studied. The comparison between BN nanotubes and

carbon nanotubes shows that BN nanotubes have more interesting characteristics for doping in carbon nanotubes[60-100].

Recently the mixing of boron nitride (BNNTs) and (CNTs) in a nanoscale particles have been investigated and these structures are made up of conical shells without any seamless. Most of the studies about these compounds have been done so far with carbon structures[55-104].

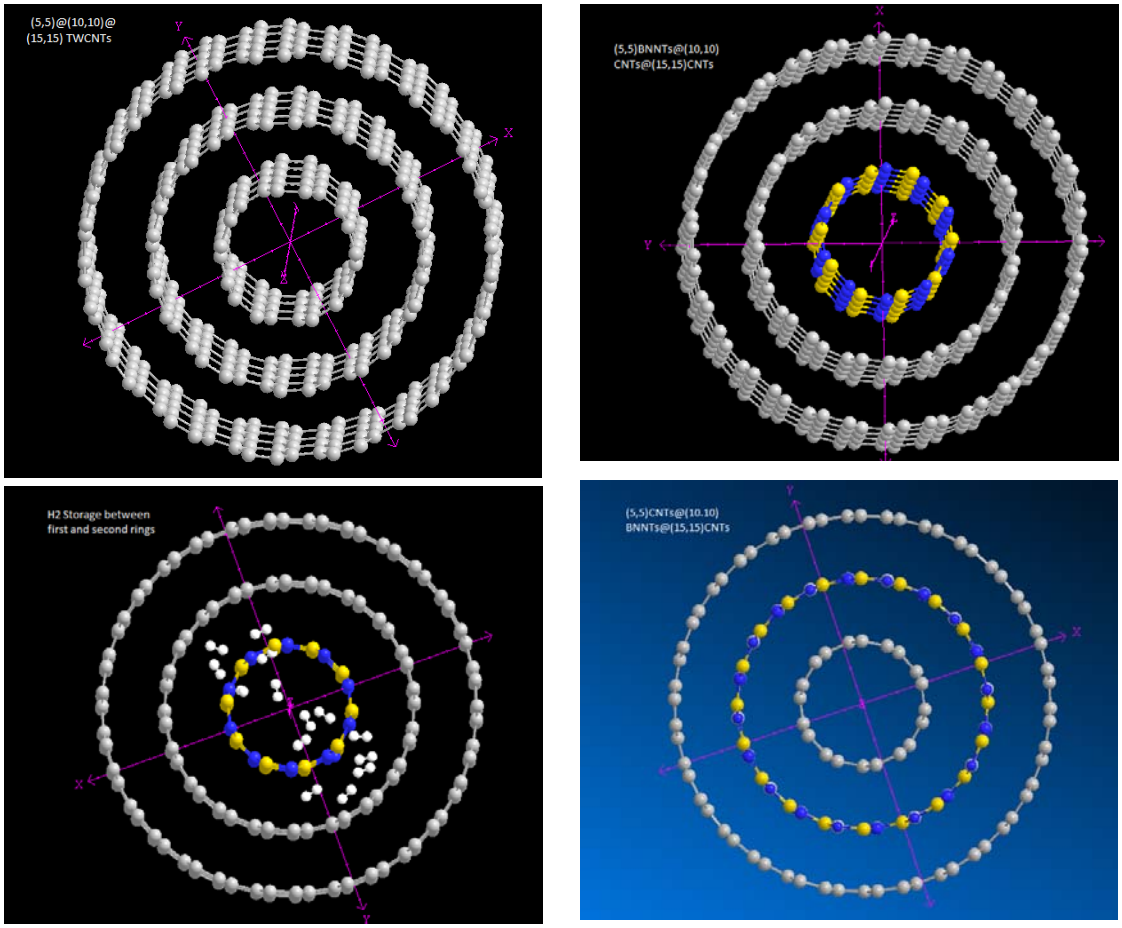
Considering the above mentioned, (BN-C) NTs nanotubes are very important and interesting for new research, especially for H2 storage and can open a huge spectrum in the field of theoretical and experimental research. In the fig.1 structure of TWCNTs is shown and this particular nanometer configuration has been proposed in this research[85-106].

Computational Method

DFT (density functional theory) is one of the computational methods which can be used in different systems and it is more useful for some calculations than other methods. It is clear that basis sets are vast various.

The Gaussian 98 program was run to obtain the best prediction of this particular structure. Also all Ab-Initio and DFT (density functional theory) calculations were done with the Gaussian 98 program. Frequency analyses were carried out to show that the optimized structures are true minima or transition states on the potential energy surfaces of a specific structure without imaginary frequencies.

In this work, geometry optimizations in the gas phase for TWCNTs were performed at density



Scheme 1: Various (5,5)@(10,10)@(15,15) TW(C&BN)NTs

functional theory (DFT) level with B3LYP and Ab-Initio with HF (hartree fock) methods in different basis sets at the temperature of 298.15K, The parameters were calculated for TWCNTs in the gas phase in different methods and basis sets include thermodynamic and NMR parameters. The chemical shielding shows the phenomenon which is dependent on the secondary magnetic field which is built by the induced movements of the electrons which encompass the nuclei. The chemical shielding is built by a three-by-three matrix which is biodegraded into a single scalar term, three antisymmetric pseudo vector components, and five components which correspond to a symmetric tensor. It can be observed the single scalar and the five symmetric tensor elements in the normal NMR spectra of the solids.

The chemical shielding tensor includes the chemical shift isotropy (CSI) and chemical shift anisotropy (CSA) and the anisotropy ($\Delta\delta$) of the tensor, the shielding tensor asymmetry parameter (η) and chemical shift (δ) are calculated.

The thermodynamic parameters that were calculated in this research are Gibbs free energy, enthalpy, internal energy (It is clear that the sum of zero point energy (ZPE) and thermal energy is internal energy.) and entropy then these reports were compared with each other in order to obtain the best results. These results were reported in tables.

RESULTS AND DISCUSSION

The results are listed in tables 1-4, and the figures are explained in figs 1-4. The geometry optimization for TWCNTs has been done with HF and B3LYP methods at different basis sets such as 4-31G, 6-31G, 6-31G* and 6-311G*. Then

Table 1: HOMO and LUMO and Gap energy of TWCNTs (atoms between, 500-540)

500(C) --> Charge:	4.000000	x,y,z(Bohr):	-17.473156	7.669501	-6.922697
501(C) --> Charge:	4.000000	x,y,z(Bohr):	-16.236503	10.027065	-6.922697
502(C) --> Charge:	4.000000	x,y,z(Bohr):	-17.966577	6.432407	-4.615341
503(C) --> Charge:	4.000000	x,y,z(Bohr):	-17.473156	7.669501	-2.307986
504(C) --> Charge:	4.000000	x,y,z(Bohr):	-18.687072	3.870157	-0.000630
505(C) --> Charge:	4.000000	x,y,z(Bohr):	-17.966577	6.432407	-0.000630
506(C) --> Charge:	4.000000	x,y,z(Bohr):	-18.911007	2.556686	2.306726
507(C) --> Charge:	4.000000	x,y,z(Bohr):	-18.687072	3.870157	4.615971
508(C) --> Charge:	4.000000	x,y,z(Bohr):	-19.083637	-0.100199	6.923327
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510(C) --> Charge:	4.000000	x,y,z(Bohr):	-19.029194	-1.431927	9.230682
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518(C) --> Charge:	4.000000	x,y,z(Bohr):	-19.083637	-0.100199	2.306726
519(C) --> Charge:	4.000000	x,y,z(Bohr):	-18.644101	-4.065998	4.615971
520(C) --> Charge:	4.000000	x,y,z(Bohr):	-19.029194	-1.431927	4.615971
521(C) --> Charge:	4.000000	x,y,z(Bohr):	-18.315596	-5.355846	6.923327
522(C) --> Charge:	4.000000	x,y,z(Bohr):	-18.644101	-4.065998	9.230682
523(C) --> Charge:	4.000000	x,y,z(Bohr):	-19.029194	-1.431927	-9.230052
524(C) --> Charge:	4.000000	x,y,z(Bohr):	-19.083637	-0.100199	-6.922697
525(C) --> Charge:	4.000000	x,y,z(Bohr):	-18.644101	-4.065998	-4.615341
526(C) --> Charge:	4.000000	x,y,z(Bohr):	-19.029194	-1.431927	-4.615341
527(C) --> Charge:	4.000000	x,y,z(Bohr):	-18.315596	-5.355846	-2.307986
528(C) --> Charge:	4.000000	x,y,z(Bohr):	-18.644101	-4.065998	-0.000630
529(C) --> Charge:	4.000000	x,y,z(Bohr):	-17.393194	-7.853133	2.306726
530(C) --> Charge:	4.000000	x,y,z(Bohr):	-18.315596	-5.355846	2.306726
531(C) --> Charge:	4.000000	x,y,z(Bohr):	-16.801441	-9.048078	4.615971
532(C) --> Charge:	4.000000	x,y,z(Bohr):	-17.393194	-7.853133	6.923327
533(C) --> Charge:	4.000000	x,y,z(Bohr):	-16.801441	-9.048078	9.230682
534(C) --> Charge:	4.000000	x,y,z(Bohr):	-18.644101	-4.065998	-9.230052
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538(C) --> Charge:	4.000000	x,y,z(Bohr):	-17.393194	-7.853133	-2.307986
539(C) --> Charge:	4.000000	x,y,z(Bohr):	-16.801441	-9.048078	-0.000630
540(C) --> Charge:	4.000000	x,y,z(Bohr):	-16.801441	-9.048078	-9.230052
Note: Orbital 1080 is HOMO, energy:		-0.223372 a.u.		-6.078253 eV	
Orbital 1081 is LUMO, energy:		-0.080224 a.u.		-2.183005 eV	
LUMO/HOMO gap:		0.143148 a.u.		3.895248 eV	375.834402 kJ/mol

thermodynamic properties were calculated for this structure in gas phase at 298.15K in the same methods and basis sets. A comparison of Gibbs free energy (G), Enthalpy (H), Entropy (S) and Internal energy (E) in different methods and basis sets are shown in table 4. As shown in table 4, the maximum values for Gibbs free-energy (G) , Enthalpy (H) and Internal energy (E) were calculated when 6-311G* basis set had been applied at B3LYP method.

HOMO and LUMO and Gap energy of TWCNTs (atoms between, 500-540) are listed in Table1.

Out Put and plot of density electron from Atoms 1-540 are shown in Fig2. Localized Orbital Locator (LOL)@Electron Localization Function ELF of (5,5)@(10,10)@(15,15) TWCNTS are shown in Fig3. Relief map and Shaded Surface map with projection for electron density of (5,5)@(10,10)@(15,15) TWCNTs in Fig4. According to the results that are shown in table2, the largest values have been obtained in B3LYP method.

Considering the optimized structure, the NMR shielding tensors were calculated then these parameters were used to show active sites in this structure. The results of σ_{iso}, $\sigma_{aniso,}$ σ, $\Delta\delta$ and η for this

Table 2: NMR Parameters of SWBNNTs @ SWCNTS

atom	σ_{ISO}	σ_{ANISO}	$\Delta\sigma$	δ	η
			4-31g		
1	71.6	179.3	179.3	119.5	0.21
2	69.1	135.3	135.3	90.2	0.27
3	154.1	75.7	75.7	50.4	0.27
4	84.5	153.2	153.2	102.1	0.07
5	30.4	333.5	333.5	222.3	0.05
6	161.4	85.1	-90.7	-60.5	0.87
7	71.9	57.8	-67.9	-45.2	0.70
8	88.5	34.2	34.2	22.8	0.70
9	83.7	120.0	120.0	80.0	0.67
10	96.7	33.4	33.4	22.3	0.39
11	-28.8	196.5	-275.9	-183.9	0.42
12	161.4	85.1	-90.7	-60.5	0.87
13	76.5	49.9	-54.7	-36.5	0.82
14	76.5	49.9	-54.7	-36.5	0.82
15	67.9	56.9	-63.0	-42.0	0.80
16	82.3	308.1	308.1	205.4	0.56
17	82.3	308.1	308.1	205.4	0.56
			6-31g		
	59.0	149.0	149.0	99.3	0.22
	61.8	191.0	191.0	127.3	0.20
	139.9	77.6	77.6	51.7	0.34
	83.7	120.0	120.0	80.0	0.67
	59.1	149.4	149.4	99.6	0.21
	151.4	90.8	-92.5	-61.6	0.96
	63.7	61.6	-72.9	-48.6	0.69
	11.9	351.6	351.6	234.4	0.03
	63.4	128.8	128.8	85.9	0.73
	88.5	34.2	34.2	22.8	0.70
	75.3	166.8	166.8	111.2	0.06
	151.4	90.8	-95.5	-64.6	0.91
	62.9	128.6	128.6	85.7	0.72
	63.4	128.8	128.8	85.9	0.73
	-27.8	194.3	-246.9	-164.6	0.66
	66.1	321.7	321.76	214.5	0.47
	66.1	321.7	321.7	214.5	0.47
			6-31g*		
1	81.9	157.2	157.2	104.8	0.07
2	77.3	121.9	121.9	81.3	0.57
3	143.1	80.9	80.9	53.9	0.30
4	92.3	34.1	34.1	22.7	0.61
5	66.9	130.8	130.8	87.2	0.25
6	157.4	85.9	85.9	57.2	1.1
7	69.3	53.5	53.5	35.6	1.4
8	26.4	337.8	337.8	225.2	0.05
9	77.3	121.9	121.9	81.3	0.57
10	92.3	34.1	34.1	22.7	0.61
11	81.9	157.9	157.2	104.8	0.07
12	157.4	85.9	85.9	57.2	1.1
13	73.4	53.8	53.8	35.8	1.1
			6-311g		
	75.1	167.0	167.0	111.3	0.06
	61.6	191.02	191.02	127.3	0.19
	139.48	76.9	76.9	51.3	0.35
	88.5	33.8	33.8	22.5	0.73
	66.7	180.3	180.3	120.	0.15
	151.4	90.9	90.9	60.6	1.0
	63.8	61.4	61.4	40.9	1.3
	12.6	350.6	350.6	233.7	0.03
	62.9	128.6	128.6	85.7	0.72
	88.5	33.8	33.8	22.5	0.73
	75.1	167.	167.0	111.3	0.06
	151.4	90.9	90.9	60.6	1.0
	68.1	57.4	57.4	38.3	1.2

nanocone in the same methods and basis sets are shown in table 3.Finally the charts of σ_{iso}, $\sigma_{aniso,}$ σ and η for the atoms of TWCNTs in the 4-31G, 6-31G, 6-31G*, 6-311G* level of theory and B3LYP and HF methods. We can obtain the interesting results from the NMR charts. Comparison of these charts (σiso, σaniso, δ and η) shows that some of peaks in these charts are similar to each other. If these peaks are reviewed, we can understand which similar atoms are situated in the same peaks of different charts. The comparison of these peaks shows that three atoms are exactly repeated in σ_{iso}, σ_{aniso}, δ and η charts. These three atoms are the active sites in this

Table 3: Some Optimized parameters

Bond-angle	6-31g	6-31g*
6-1-18	147.91	143.74
3-2-8	140.64	140.5
2-3-4	101.0	101.5
2-3-10	101.0	101.5
4-3-10	90.29	91.19
3-4-6	112.1	112.7
3-4-14	118.9	117.74
6-4-14	119.8	119.2
6-5-12	153.9	150.4
1-6-4	100.2	101.8
1-6-5	116.1	118.4
4-6-5	94.3	96.0
8-7-9	119.8	120.5
8-7-14	119.8	120.5
9-7-14	109.0	106.4
1-6	1.444	1.469
1-18	1.279	1.283
2-3	1.423	1.449
2-8	1.296	1.309
3-4	1.549	1.567
3-10	1.549	1.567
4-6	1.605	1.599
4-14	1.419	1.442
5-6	1.366	1.389
5-12	1.366	1.389
7-8	1.456	1.463
7-9	1.539	1.560
7-14	1.539	1.560
9-10	1.419	1.442
9-16	1.544	1.556

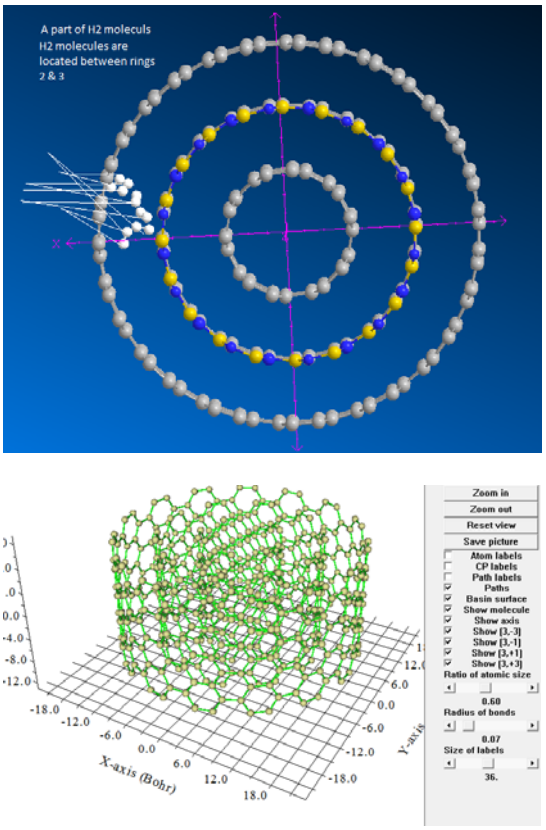

Fig. 1: The optimized structures of 3 Nano Cone including H2 storage

Table 4: Thermodynamic properties in different methods and basis sets, for TWCNTs without and including H2 at 298.15K in gas phase

Methods	Basis set	Relative E(kcal/mol) -	-G(kcal/mol) Relative	H(kcal/mol)- Relative
	4-31g	0	0	0
B3LYP	6-31g	5.35	6.33	3.99
	6-31g*	7.22	5.55	5.05
	6-311g*	4.25	4.96	7.22
Including H2	6-31g*	8.67	9.772	7.99

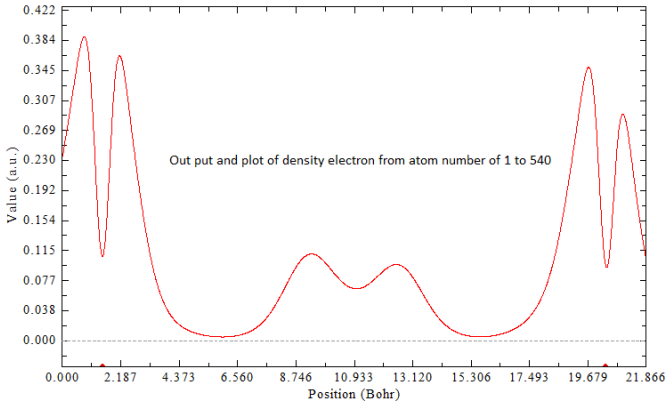

Fig. 2: Out Put and plot of density electron from Atoms 1-540

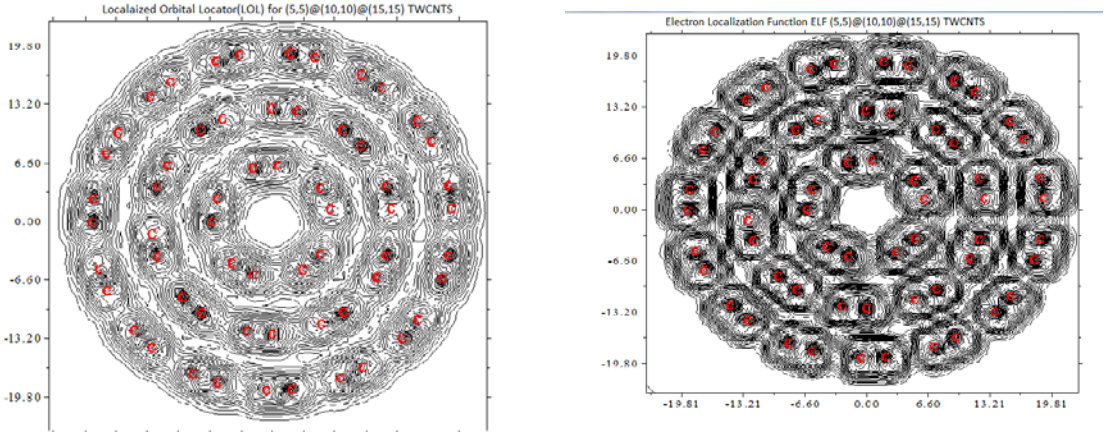

Fig. 3: Localized Orbital Locator (LOL)@Electron Localization Function ELF of (5,5)@(10,10)@(15,15) TWCNTS

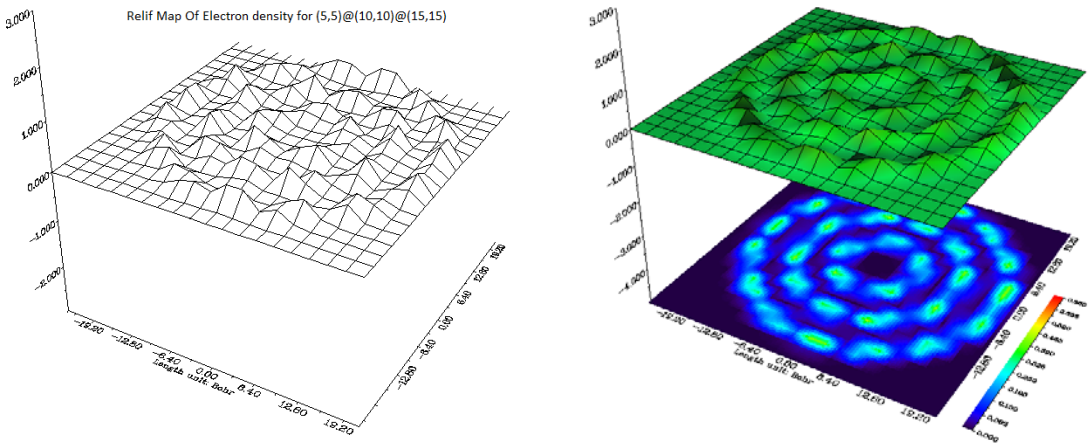

Fig. 4: Relief map and Shaded Surface map with projection for electron density of (5,5)@(10,10)@(15,15) TWCNTs

structure in TWCNTs and SWBNNTs @ DWCNTs. In general, the chart of electronic charge in different methods and basis sets is similar to the charts of NMR parameters Nitrogen atoms have more electrons than Boron atoms therefore the location of negative electronic charge is on Nitrogen atoms and positive electronic charge is situated on Boron atoms. It is clear that Nitrogen atoms will be active sites in this structure.

CONCLUSION

In summary, the stability of TWCNTs and SWBNNTs @ DWCNTs were investigated. It is found that the amount of Gibbs free energy (G) , Enthalpy (H) and internal Energy (E) obtained in B3LYP/6-311G* level in the gas phase (298.15K) are the largest amount and also optimization of TWCNTs and SWBNNTs @ DWCNTs at the B3LYP/ 6-311G*is suitable for this structure. The NMR data and the thermodynamics results indicate that this kind of nano-structures is suitable for H2 Storage.

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