Deuterium adsorption on Multi Carbon Nano-cone (MNC$_x$, X=2-7) including BN Nano-cone: A model for D$_2$ storage

SEPIDEH MORADI

Department of Chemistry, Science and research branch, Islamic Azad University, Tehran, Iran
*Corresponding author E-mail: sepideh.mm92@yahoo.com

ABSTRACT

A mixing of Multi Wall (BN&C) Nano-cones have been modeled and calculated for the suitable structures to storage the Deuterium molecules. We have found these kinds of nano-structures are useful for maximum storages of D2 molecules. B3LYP/6-31G/6-31G/6-31G*/6-31+G* density functional theory (DFT) calculations have performed for the structure and stability of two, three, four and seven wall (BN&C) Nano-cones. In this work, it was calculated the geometrical structure, and stability to predict NMR and NBO parameters.

Key words: Storages of D2 molecule, Density functional theory (DFT), Ab-initio calculation, Thermodynamic parameters.

INTRODUCTION

Deuterium is one of two stable isotopes of hydrogen. The nucleus of deuterium, called a deuteron, contains one proton and one neutron, whereas the far more common hydrogen isotope, protium, has no neutron in the nucleus.

Deuterium is destroyed in the interiors of stars faster than it is produced. Other natural processes are thought to produce only an insignificant amount of deuterium. Theoretically nearly all deuterium found in nature was produced in the Big Bang 13.8 billion years ago, as the basic or primordial ratio of hydrogen-1 (protium) to deuterium (about 26 atoms of deuterium per million hydrogen atoms) has its origin from that time. This is the ratio found in the gas giant planets, such as Jupiter[1-3].

Although much study has been done for nanotube carbon phenomenon[4-12], there are a few studies for Multi Nano-cone. The carbon nanotube (CNT) is a representative nano-material. CNT is a cylindrically shaped carbon material with a nano-metric-level diameter[4-17].

Carbon nano cone has a high asymmetric geometry that in our simulations, classical non-equilibrium molecular dynamics method is adopted.

The cone is entirely characterized by its cone angle. When one pentagon is introduced into a hexagonal carbon network, a 60 declination defect is formed; leading to the formation of a nano cone with cone angle of 118 and the equilibrium carbon-carbon bond length is 1.418 Å. In this work, we focus on the cone with the cone angle of 180, which is the largest angle observed experimentally and theoretically. Moreover, in all theoretical models so far, the rectification efficiency decreases quickly as the structure length increases.

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[5-22].

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[10-25].

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[20-35].

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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[37-45].

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 [40-50]. 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[48-55].

Boron nitride nanotube (BNNTs) have attracted much interests due to their large gap semi conducting character[49-60].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[54-64], carbon nanotube templates[50-66], and laser ablating[59-69] 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[61-77].

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[65-85].

The most stable TWC-Nano-cones structure is built from[75-104].In this work, we have focused on MWC-Nano-cones and double Wall C - (BN) nano-con. Our aim was to obtain the global minimum energy structure. For this structure, we use the QM/MM methods of 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 MWC-Nano-cones is shown and this

particular nanometer configuration has been proposed in this research[85-106].

Computational Method

In this work, 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.

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. geometry optimizations in the gas phase for MWC-Nano-cones were performed at density 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 MWC-Nano-cones 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 tensor includes the chemical shift isotropy (CSI) and chemical shift anisotropy (CSA) and the anisotropy ($\Delta\eta$) of the tensor, the shielding tensor asymmetry parameter (σ) and chemical shift (δ) are calculated.

The chemical shift refers to phenomenon which associated with the secondary magnetic field created by the induced motions of the electrons that surrounding the nuclei when in the presence

of an applied magnetic field. .. The shielding ó, is the differential resonance shift due to the induced motion of the electrons. The chemical shielding tensor is commonly referred to the chemical shift anisotropy (CSA) tensor according to the possession of second rank properties. The CSA tensor can be described by three additional parameters.

a)   The isotropic value (δ_{iso}), of the shielding tensor which can be defined as[59-61].

$$\sigma_{iso} = \frac{1}{3}(\sigma_{11} + \sigma_{22} + \sigma_{33})$$

b) The chemical shift anisotropy parameter ("ó), due to the following expression:

$$\text{if } |\sigma_{11} - \sigma_{iso}| \geq |\sigma_{33} - \sigma_{iso}| \quad | \Delta\sigma = \sigma_{11} - \frac{\sigma_{22}+\sigma_{33}}{2}$$

$$\text{if } |\sigma_{11} - \sigma_{iso}| \leq |\sigma_{33} - \sigma_{iso}| \quad \Delta\sigma = \sigma_{33} - \frac{\sigma_{22}+\sigma_{11}}{2}$$

and

$$\text{If } |\sigma_{11} - \sigma_{iso}| \geq |\sigma_{33} - \sigma_{iso}| \quad \eta = \frac{\sigma_{22}-\sigma_{33}}{\delta}$$

$$\text{If } |\sigma_{11} - \sigma_{iso}| \leq |\sigma_{33} - \sigma_{iso}| \quad \eta = \frac{\sigma_{22}-\sigma_{11}}{\delta}$$

c) The asymmetry parameter (•), which has given by:

$$\Omega = \sigma_{33} - \sigma_{11}$$

It is useful to define the span (Ù), and the skew (8) of a CSA tensor. The span is defined

$$\kappa = \frac{3(\sigma_{iso} - \sigma_{22})}{\Omega}$$

And indicates the width of the NMR line shape for a nonspinning, stationary, sample . The skew is defined as:

RESULTS AND DISCUSSION

The results are listed in tables 1-3, and the figures are explained in figs 1-4. The geometry optimization for Multi Nano-cone (MNC$_x$, X=2-7) including BN doping have been done with HF and B3LYP methods at different basis sets such as 4-31G, 6-31G, 6-31G* and 6-31+G*. Then

thermodynamic properties were calculated for this structure in gas phase at 298.15K in the same methods and basis sets.

HOMO and LUMO and Gap energy of MWC-Nano-cones (atoms between, 520-560) are listed in Table1.

Relief map and Shaded Surface map with projection for electron density of 7 Nano-cone of Multi Nano-cone (MNC$_x$, X=2-7) are shown in Fig1.

Out Put and plot of density electron from Atoms 1-560 are shown in Fig2. Localized Orbital Locator (LOL)@Electron Localization Function ELF of Multi Nano-cone (MNC$_x$, X=2-7) including BN doping are shown in Fig1.

The situation of Deuterium adsorption between two nano cones and The situation of Deuterium adsorption between two nano cones 1-BN 2-Carbon are shown in Fig3 and Fig4 .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}, σ_{aniso}, σ, Äα and Δ for this nanocone in the same methods and basis sets are shown in table 3.Finally the charts of σ_{iso}, σ_{aniso}, η and ç for the atoms of Multi Nano-cone (MNC$_x$, X=2-7) including BN doping in the 4-31G, 6-31G, 6-31G*, 6-31+G* level of theory and B3LYP and HF methods. We can obtain the interesting results from the NMR charts. Comparison of these charts (áiso, áaniso, ä and ç) 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}, σ and δ charts.These three atoms are the active sites in this structure in Multi Nano-cone (MNC$_x$, X=2-7) including BN doping. 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.

Table 1: HOMO and LUMO and Gap energy of Nano-cone including 7 layers (between, atoms 520 - 560)

```
520(C ) --> Charge:   4.000000  x,y,z(Bohr):   -4.854612   40.551279    6.366487
521(C ) --> Charge:   4.000000  x,y,z(Bohr):   -3.592275   42.915326    2.609712
522(C ) --> Charge:   4.000000  x,y,z(Bohr):   -3.031026   41.964794    5.032341
523(C ) --> Charge:   4.000000  x,y,z(Bohr):   -1.797035   44.389313    1.305801
524(C ) --> Charge:   4.000000  x,y,z(Bohr):    0.686065   44.389313    2.110824
525(C ) --> Charge:   4.000000  x,y,z(Bohr):    0.686065   44.389313   -2.110824
526(C ) --> Charge:   4.000000  x,y,z(Bohr):    2.220523   44.389313   -0.000000
527(C ) --> Charge:   4.000000  x,y,z(Bohr):    1.372036   42.915326   -4.223538
528(C ) --> Charge:   4.000000  x,y,z(Bohr):    3.849467   41.964794   -4.438967
529(C ) --> Charge:   4.000000  x,y,z(Bohr):    2.743977   39.969243   -8.447076
530(C ) --> Charge:   4.000000  x,y,z(Bohr):    4.554335   40.551279   -6.583806
531(C ) --> Charge:   4.000000  x,y,z(Bohr):    3.429948   38.497146  -10.557900
532(C ) --> Charge:   4.000000  x,y,z(Bohr):    5.943283   37.659998  -10.839469
533(C ) --> Charge:   4.000000  x,y,z(Bohr):  -11.444087   38.068179    2.656955
534(C ) --> Charge:   4.000000  x,y,z(Bohr):  -11.179525   37.659998    5.276115
535(C ) --> Charge:   4.000000  x,y,z(Bohr):   -9.586486   39.442010    1.330367
536(C ) --> Charge:   4.000000  x,y,z(Bohr):   -7.555030   40.551279    2.649396
537(C ) --> Charge:   4.000000  x,y,z(Bohr):   -5.721996   41.964794    1.328477
538(C ) --> Charge:   4.000000  x,y,z(Bohr):   -3.592275   42.915326   -2.609712
539(C ) --> Charge:   4.000000  x,y,z(Bohr):   -1.797035   44.389313   -1.305801
540(C ) --> Charge:   4.000000  x,y,z(Bohr):   -3.031026   41.964794   -5.032341
541(C ) --> Charge:   4.000000  x,y,z(Bohr):   -0.504462   41.964794   -5.852482
542(C ) --> Charge:   4.000000  x,y,z(Bohr):   -1.696879   39.442009   -9.527999
543(C ) --> Charge:   4.000000  x,y,z(Bohr):    0.185288   40.551279   -8.002990
544(C ) --> Charge:   4.000000  x,y,z(Bohr):   -1.009019   38.068179  -11.706853
545(C ) --> Charge:   4.000000  x,y,z(Bohr):    1.562898   37.659998  -12.264323
546(C ) --> Charge:   4.000000  x,y,z(Bohr):  -13.439637   36.902218    1.332257
547(C ) --> Charge:   4.000000  x,y,z(Bohr):   -7.555030   40.551279   -2.649396
548(C ) --> Charge:   4.000000  x,y,z(Bohr):   -5.721996   41.964794   -1.328477
549(C ) --> Charge:   4.000000  x,y,z(Bohr):   -7.184644   39.969243   -5.221313
550(C ) --> Charge:   4.000000  x,y,z(Bohr):   -4.854612   40.551279   -6.366487
551(C ) --> Charge:   4.000000  x,y,z(Bohr):   -6.064036   38.068179  -10.062792
552(C ) --> Charge:   4.000000  x,y,z(Bohr):   -4.229112   39.442010   -8.705968
553(C ) --> Charge:   4.000000  x,y,z(Bohr):   -5.419640   36.902218  -12.372037
554(C ) --> Charge:   4.000000  x,y,z(Bohr):   -2.887407   36.902218  -13.194068
555(C ) --> Charge:   4.000000  x,y,z(Bohr):  -11.444087   38.068179   -2.656955
556(C ) --> Charge:   4.000000  x,y,z(Bohr):   -9.586486   39.442010   -1.330367
557(C ) --> Charge:   4.000000  x,y,z(Bohr):  -11.179525   37.659998   -5.276115
558(C ) --> Charge:   4.000000  x,y,z(Bohr):   -8.981774   38.497146   -6.525224
559(C ) --> Charge:   4.000000  x,y,z(Bohr):   -8.473437   37.659998   -9.002655
560(C ) --> Charge:   4.000000  x,y,z(Bohr):  -13.439637   36.902218   -1.332257
Note: Orbital  1120 is HOMO, energy:   -0.244389 a.u.    -6.650155 eV
      Orbital  1121 is LUMO, energy:   -0.063073 a.u.    -1.716304 eV
      LUMO/HOMO gap:      0.181316 a.u.     4.933851 eV      476.044336 kJ/mol
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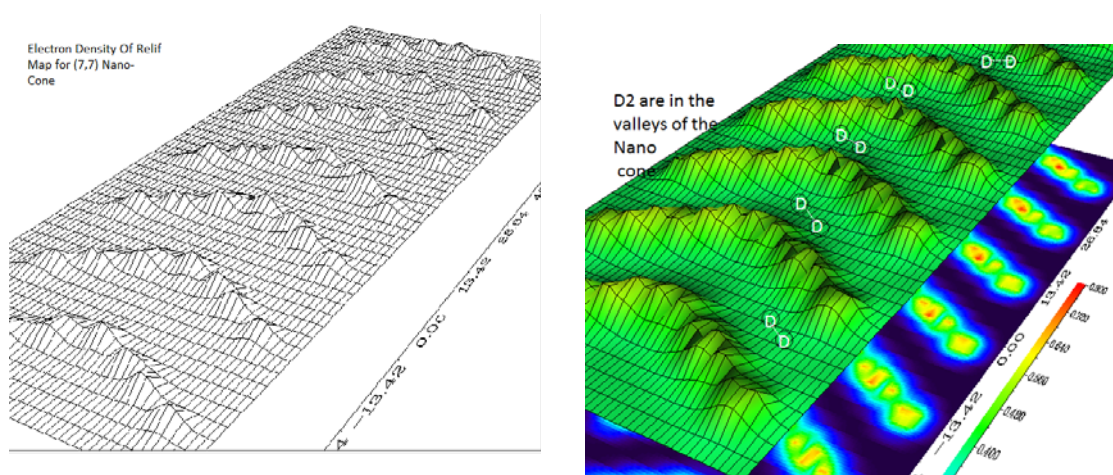

Electron Density Of Relif Map for (7,7) Nano-Cone

D2 are in the valleys of the Nano cone

Fig. 1: Relief map and Shaded Surface map with projection for electron density of 7 Nanocone

Fig. 2: The electron density distribution of 7 Nano-cone

Fig. 3: The situation of Deuterium adsorption between two nano cones
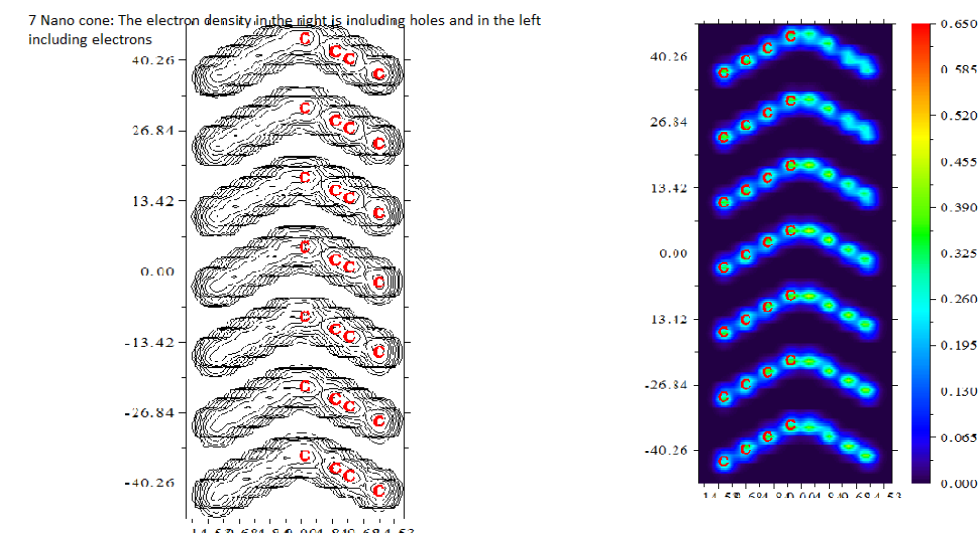
Table 2: NMR Parameters of SWBNNTs @ SWCNTS6-31g

Atom	σ_{ISO}	σ_{ANISO}	$\Delta\sigma$	δ	η
6-31g					
1	143.1	80.9	80.9	53.9	0.3
2	88.5	33.8	33.8	22.5957	0.7
3	83.7	120.0	120.0	80.0	0.67
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	63.7	61.67	-72.9	-48.6	0.69
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	81.9	157.9	157.2	104.8	0.07
15	75.1	167.0	167.0	111.3	0.06
16	61.6	191.02	191.02	127.3	0.19
17	139.48	76.9	76.9	51.3	0.35
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
	75.3	166.8	166.8	111.2	0.06
	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
	96.7	33.4	33.4	22.3	0.39
	62.9	128.6	128.6	85.7	0.72
	88.5	33.8	33.8	22.5	0.73
	63.4	128.8	128.8	85.9	0.73
	151.4	90.9	90.9	60.6	0.99
	63.4	128.8	128.8	85.9	0.73
	92.3	34.1	34.1	22.7	0.61
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	-27.8	194.3	-246.9	-164.6	0.66
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	75.1	167.	167.0	111.3	0.06
11	30.4	333.5	333.5	222.3	0.05
6+31g*					
	66.1	321.7	321.7	214.5	0.47
	82.3	308.1	308.1	205.4	0.56
	82.3	308.1	308.1	205.4	0.56
	88.5	33.8	33.8	22.5	0.73
	76.5	49.9	-54.7	-36.5	0.82
	157.4	85.9	85.9	57.2	0.99
	151.4	90.9	90.9	60.6	0.99
	12.6	350.6	350.6	233.7	0.03
	151.4	90.8	-95.5	-64.6	0.91
	62.9	128.6	128.6	85.7	0.72
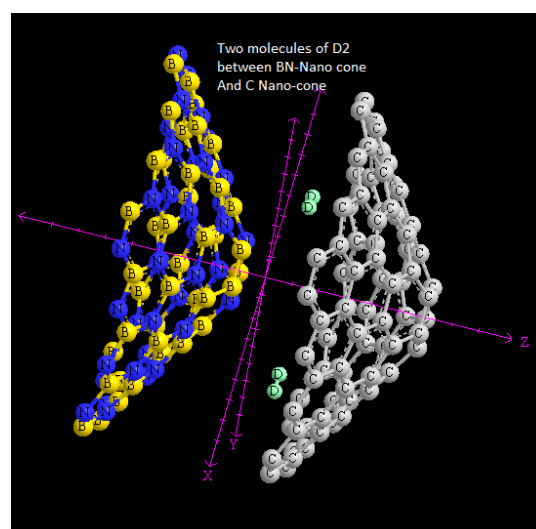
Fig 4: The situation of Deuterium adsorption between two nano cones 1-BN 2-Carbon

CONCLUSION

In summary, the stability of MWC-Nano-cones 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/6-31+G* level in the gas phase (298.15K) are the largest amount and also optimization of MWC-Nano-cones and SWBNNTs @ DWCNTs at the B3LYP/6-31+G*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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