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NMR Shielding Tensors and Thermodynamic Investigation of $B_{28}N_{28}$ Nano-cone Structure: A molecule for Fe^{3+}Capturing

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ABSTRACT

M06&B3LYP/3-21G/6-31G/6-31G*/6-311G* density functional theory (DFT) and HF/3-21G/6-31G/6-31G*/6-311G *ab-initio calculations have performed for the structure and stability of $B_{28}N_{28}$ nano-cone. In this work, it was calculated the geometrical structure, and stability to predict NMR and thermodynamics parameters. We have found these kinds of nano-cone are useful for capturing of Fe3+ Ion

Key words: Fe^{3+} Ion, Density functional theory (DFT), Ab-initio calculation, Geometrical structure, Thermodynamic parameters, Active sites.

INTRODUCTION

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. Primarily discovery of C60 has led to synthesizing higher fullerenes, carbon nanotubes, and other non-carbon nanostructures such as BN nanotubes .Although BN neocons have been known since 1994, we have been able to observe these structures experimentally until recently[1-6].

The carbon nanotube (CNT) is a representative nano-material. CNT is a cylindrically shaped carbon material with a nano-metric-level diameter[10-20].

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[6-15].

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[16-20].

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].

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. 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[20-26].

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[25-40]. Two years later single walled nanotubes were reported[8-15]. 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[30-50].

boron nitride nanotube (BNNTs) have attracted much interests due to their large gap semi conducting character[41-55].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[44-60], carbon nanotube templates[50-65], and laser ablating[52-64]. 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. Jensen and Toftlund[58-70] performed *ab initio* calculations for B28N28,c sters in different geometries**.** Based on density functional calculations it has also been proposed that other nanotube could be synthesized[60-75].

Theoretical studies have been performed for fullerene-like B28N28 clustersin 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 B28N28structure is built from six squares and eight hexagons[70-102].

In this work, we focused on B*28*N*28* 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-cones are useful for Fe^{3+}Capturing. 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. The BN cluster is a polar molecule and BN 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 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 than the carbon nanotubes[60-100].

Recently the boron nitride (BN) nanoscale cone particles have been discovered and these structures are made up of conical shells without any seamless. Most of the studies about nanocones have been done so far with carbon structures. High-resolution transmission electron microscopy and nanobeam electron diffraction made the orientation of the BN hexagonal rings possible. Recently theoretical investigations on (BN) n nanocones have gained more attention in carbon nanotubes when there is not any experimental result [55-100].

Considering the above mentioned, BN nanotubes are very important and interesting for new research and can open a huge spectrum in the field of theoretical and experimental research. In the fig.1 structure of $B_{28}N_{28}$ is shown and this particular nanocone configuration has been proposed in this research.

Computational Method

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 $B_{28}N_{28}$ 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 $B_{28}N_{28}$ 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 ($\Delta\sigma$) 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 1-3, and the figures are explained in figs 1-4. The geometry optimization for $B_{28}N_{28}$ nano-cone has been done with HF and B3LYP methods at different basis sets such as 4-31G, 6-31G, 6-31G* and 6-311G*. Then 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 2. As shown in table 2, 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.

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}, $\sigma_{aniso,}$ δ, η and · for this nanocone in the same methods and basis sets are shown in table 3.Finally the charts of σ_{iso}, $\sigma_{aniso,}$ δ and η for the atoms of $B_{10}N_{11}$ 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 (σ_{iso}, σ_{aniso}, 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 σ charts. These three atoms are the active sites in this structure in $B_{28}N_{28}$

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

Table 1: HOMO and LUMO and Gap energy of 3 N28B28 Nanocone

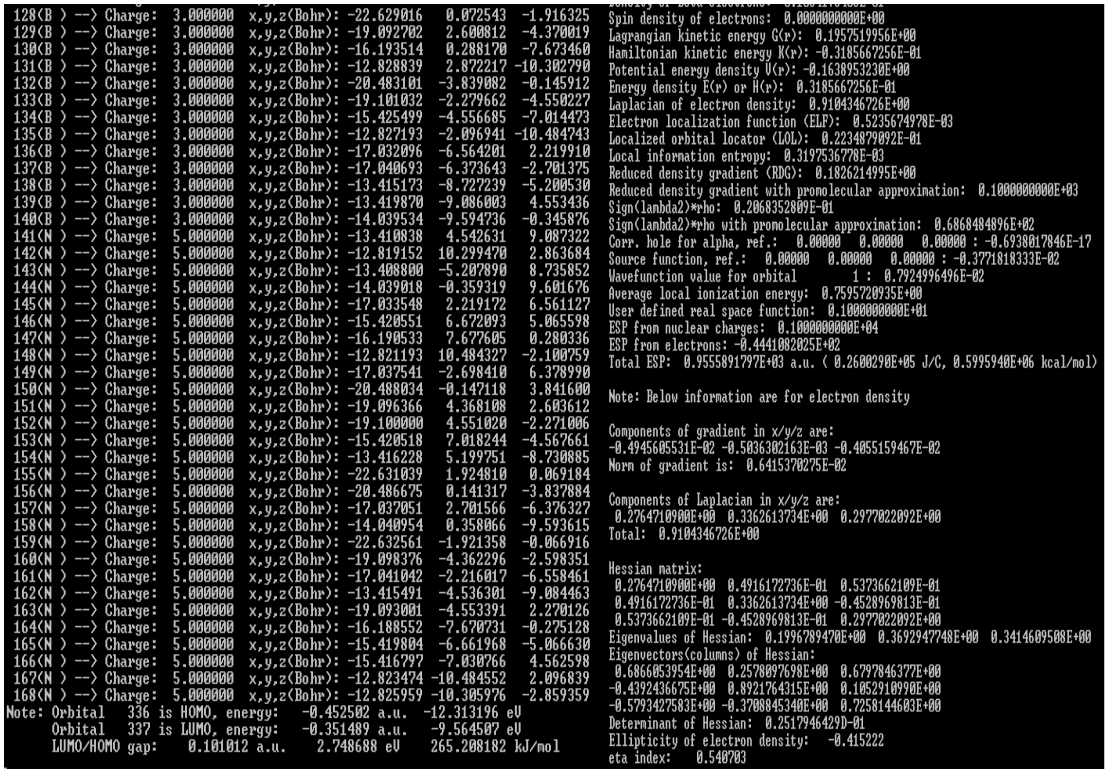

Table 2: Thermodynamic properties in different methods and basis sets, for B28N28 without and including Fe^{3+} at 298.15K in gas phase)

Methods	Basis set	Relative E(kcal/mol)	-G(kcal/mol) Relative	H(kcal/mol)- Relative
	4-31g	0	0	0
HF	6-31g	2.25	2.33	1.99
	6-31g*	3.32	3.55	2.05
	6-311g*	3.45	3.96	3.22
	4-31g	0	0	0
B3LYP	6-31g	3.33	2.55	1089
Including Fe^{3+}	6-31g*	3.62	3.13	2.77
	6-311g*	3.99	4.01	3.43
	6-31g*	5.66	6.22	5.34

Table 3: NMR parameters: including for $B_{28}N_{28}$ in different methods and basis sets

Methods		*HF* B3LYP										
	Atoms	**100N**	**101N**	**1B**	**102N**	**10B**	**20B**	**Fe3+**	**17N**	**28B**	**150N**	**168N**
4-31g	σ_{iso}	104.6	158.5	105.7	183.8	101.1	96.68	178.58	178.59	129.73	158.4	104.68
		110.2	96.7	98.3	154. 8	95. 5	88. 6	157.44	157.46	91.3	96.3	105.2
	σ_{aniso}	168	29.63	52.5	158. 0	129. 3	82	84. 1	84.78	115.7	29.9	168
		164.9	60.9	47.1	159. 9	114. 5	66. 0	103.58	103.54	115.7	60.6	164.09
	$\Delta\sigma$	168	-41.7	-70.5	158.9	129.6	82.98	84.75	84.75	115.73	-41.9	168.05
		164.6	-61.7	-62. 5	159.89	114. 6	66. 3	103.59	103.5	113.7	-61.4	164. 1
	η	0.44	0.46	0.57	0.26	0.153	0.51	0.54	0.54	0.45	0.41	0.44
		0.94	0.99	0.53	0.24	0.32	0.87	0.166	0.162	0.616	0.96	0.91
	δ	1125	-27. 8	-46. 8	105. 3	86.4	55.3	56.54	56.55	77.1	-27.9	112.03
		109.4	-40.5	-41. 9	106. 6	76.26	44.47	69.06	69	75.4	-40. 6	109.9
6-31g	σ_{iso}	165.6	165. 9	88.2	168. 4	80.4	92	104.53	145. 4	78. 9	145. 6	92.04
		139.8	139.1	88. 5	136. 5	83.3	-20.7	64.24	78.31	77. 2	78. 3	-20.68
	σ_{aniso}	96.3	96.3	60.2	176. 4	155.5	173.9	130.1	46.9	99. 6	46. 8	173.1
		113.2	113.5	54.52	179. 2	126.7	179.06	135.5	59.6	76. 0	59.48	179.06
	$\Delta\sigma$	96.3	96.3	-79.9	176.8	155.59	173.9	130.1	-52.6	99.4	-52.05	173. 1
		113.2	113. 4	-70.3	179.61	126.71	179.03	135.5	-59.5	76.5	-59.5	179. 6
	η	0.45	0.44	0.5	0.26	0.19	0.51	0.368	0.76	0.57	0.783	0.51
		0.15	0.16	0.54	0.2	0.33	0.793	0.53	0.96	0.8	0.99	0.799
	δ	64.2	64.2	-53.3	117.27	103.6	115.9	86. 1	-35. 9	66.37	-35. 7	115.9
		75.4	75. 1	-47. 8	119.7	84.5	119.3	90. 9	-39.6	50. 7	-39. 7	119.3
6-31g*	σ_{iso}	102. 4	164.19	172. 9	172. 7	88. 7	85. 5	126. 7	183.4	155.21	165.26	94.05
		30.63	109.56	148. 4	148.12	83.3	75.55	86. 0	152.03	129.1	109.57	84. 9
	σ_{aniso}	174.74	45.19	93.02	93.06	155	95. 1	127.7	170. 9	97.3	45.18	56.6
		172.19	46. 4	106. 1	106. 2	141.8	85	125.5	171	114.6	46. 6	54.29
	$\Delta\sigma$	174.7	-62.45	93.09	93	155. 5	95. 2	127.7	170.8	97.3	-62. 7	-76.2
		172.16	46.2	106. 9	106.6	141. 5	85.04	125.5	171	114. 7	46. 6	-71. 3
	η	0.526	0.44	0.41	0.45	0.147	0.56	0.43	0.35	0.47	0.445	0.48
		0.452	0.186	0.28	0.242	0.25	0.69	0.48	0.3	0.21	0.1868	0.57
	δ	116. 6	-41. 9	62. 7	62	103.4	63. 5	85. 3	113. 7	64. 50	-41. 8	-50. 67
		114.7	30. 3	71. 7	71.1	94.3	56.6	83. 7	114	76. 1	30. 1	-47. 5
6-311g*	σ_{iso}	82.31	102.3	86.9	167.4	79.5	76.93	106.2	155.2	82. 6	147.8	147.89
		4.3	30.4	74.9	132	71.1	63.6	61.6	129.19	4.3	89	89.3
	σ_{aniso}	186.1	174.6	62.9	178.13	167.5	103.7	129.4	97.35	186.6	49.8	49.8
		186. 4	172	60.9	184.6	156.25	94.83	132.4	114.4	186.97	50.14	50.11
	$\Delta\sigma$	186.6	174.7	-81.6	178.3	167.5	103.3	129.7	97.3	186.6	-67.5	-67.56
		186.9	172.1	-78.9	184.2	156.2	94.8	132.26	114. 5	186.9	50.1	50.2
	η	0.5	0.5	0.59	0.36	0.14	0.52	0.46	0.49	0.51	0.47	0.47
		0.48	0.45	0.54	0.3	0.21	0.68	0.49	0.22	0.41	0.13	0.13
	σ	124.4	116.4	-54. 0	118. 5	111.7	68. 4	86. 2	64.9	124. 9	-45	-45.04
		124.64	114.76	-52.6	123.08	104.16	63.27	88.19	76. 76	124.6	33.43	42.4

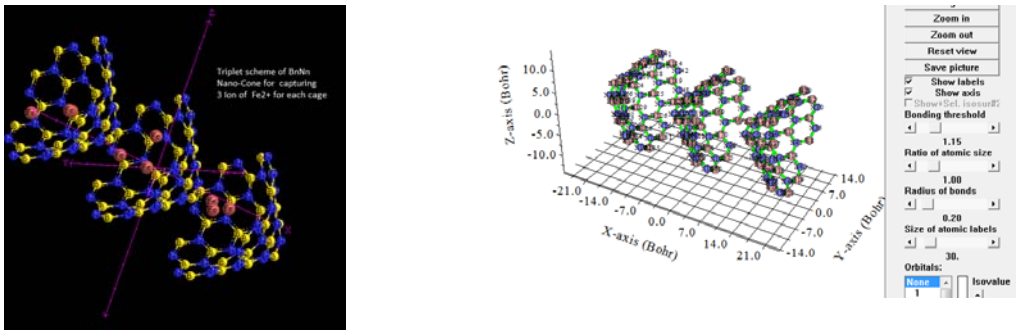

Fig 1: The optimized structures of 3 Nano Cone including Fe^{3+} Ion capturing

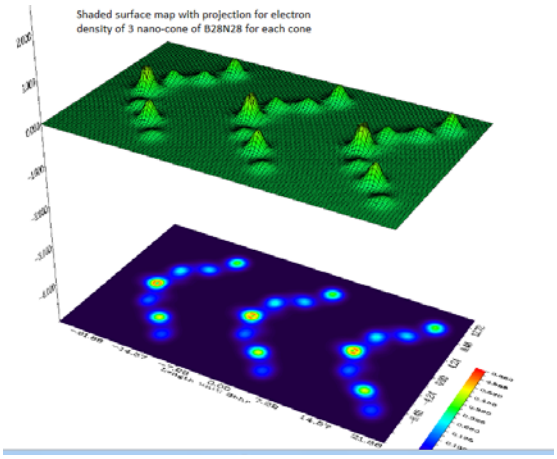

Fig. 2: Shaded Surface map with projection for electron density of 3 nano-cone of B28N28

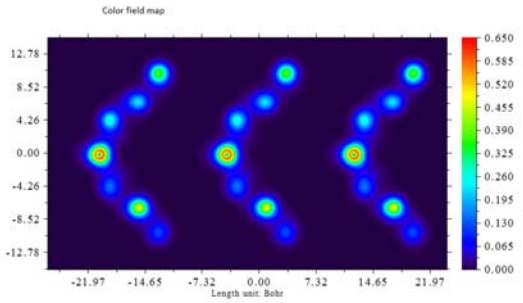

Fig. 3: Color map of 3 28N28 shows the most density in top of each nano-cone

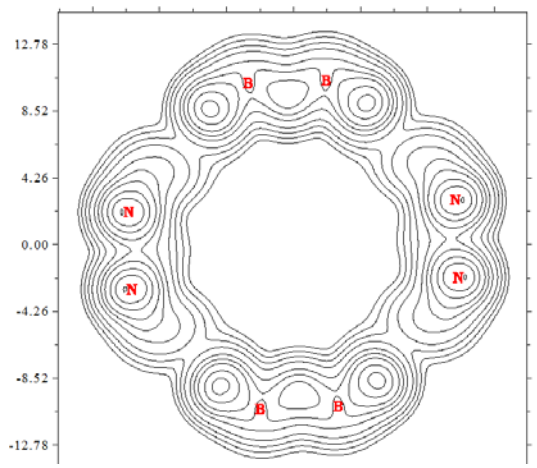

Fig. 4: The line of contour map

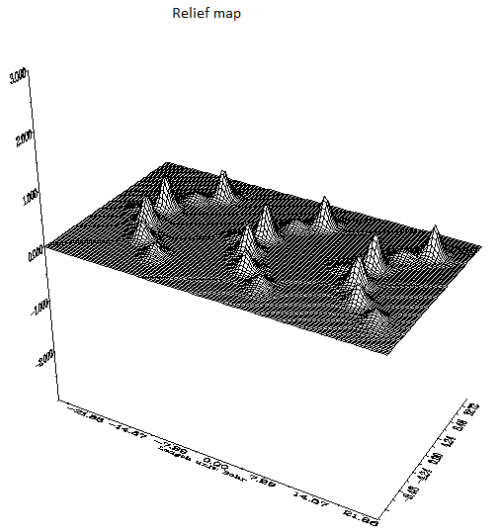

Fig. 5: Relief map shows the situation of 3 nano-cones versus distance

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 $B_{28}N_{28}$ was 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 $B_{28}N_{28}$ nano-cone at the B3LYP/6-311G*is suitable for this structure. The NMR data and the thermodynamics results indicate that this kind of nano-cone is suitable for capturing Fe^{3+} ion.

REFERENCES

1. Kroto, H. W.; Health, J. R.; O'Brien, S. C.; Curl, R. F.; Smalley, R. E. C60: *Buckminsterfullerene. Nature (London)*, **1985**, *318*, 162
2. Iijima Sumio*. Nature* (*London*), **1991**. 354, 56.
3. Chopra, Nasreen G.; Luyken , R. J.; Cherrey , K.; Crespi , Vincent H.; Cohen, Marvin L.; Louie, Steven G.; Zettl , A. *Science*,**1995**, *269*, 966.
4. Rubio Angel; Corkill , Jennifer L.; Cohen , Marvin L. *Phys. Rev*. **1994**. B, *49*, 5081
5. Bourgeois,L.; Bando,Y.; Han, W.Q.; Sato, T.*Phys. Rev*. **2000**, B, *61*, 7686.
6. Terauchi, M.; Tanaka, K.; Suzuki, A.; Ogino, K.; Kimura, Chem. Phys. Lett. **2000**, 324, 359.
7. Sachdeva, H, Frank Müllera, F .; Stefan Hüfnerb, S. Diamond and Related Materials, 2010. 19, 1027-1033.
8. Massimo, Fusaro .:*Quantum Matter,**2014,** 3*, 481-487
9. Micheal Arockiaraj , Rev. *Theor. Sci*. **2014**, *2*, 261-273
10. Martin Bohlén .; Kim Bolton ,*Quantum Matter*, **2014**, *3*, 339-343
11. Monajjemi, M.; Baei, M.T.; Mollaamin, F. *Russian Journal of Inorganic Chemistry.* **2008,** *53 (9),* 1430-1437
12. Monajjemi, M.; Rajaeian, E.; Mollaamin, F.; Naderi, F.; Saki, S. *Physics and Chemistry of Liquids.* **2008**, *46 (3)*, 299-306
13. Monajjemi, M.; Seyed Hosseini, M. *Journal of Computational and Theoretical Nanoscience* .**2013** ,*10 (10)*, 2473-2477
14. Yahyaei ,H.; Monajjemi, M. *Fullerenes, Nanotubes, and Carbon Nanostructures*.**2014**, *22(4)*, 346–361
15. Monajjemi, M .; Jafari Azan, M.; Mollaamin, F. *Fullerenes, Nanotubes, and Carbon Nanostructures*.**2013**, *21(6)*, 503–515
16. Bhupesh, Bishnoi .; Bahniman ,Ghosh .*Quantum Matter*.**2014,** *3*, 469-475
17. Sule, Celasun , Rev. *Theor. Sci*.**2013,** *1*, 319-343
18. Akshaykumar, Salimath .; Bahniman, Ghosh, *Quantum Matter,* **2014,** 3, 72-77
19. Nafisi, S.; Monajemi, M.; Ebrahimi, S. *Journal of Molecular Structure*. **2004**,*705 (1-3)* 35-39
20. Monajjemi , M.; Baheri ,H.; Mollaamin ,F. *Journal of Structural Chemistry*.**2011** 52(1), 54-59
21. Monajjemi, M.; Seyed Hosseini, M.; Mollaamin, F. *Fullerenes, Nanotubes, and Carbon Nanostructures*. **2013,** 21, 381–393
22. Monajjemi, M.; Boggs, J.E. *J. Phys. Chem. A*, **2013,** *117,* 1670 "1684
23. Davide Fiscaletti and Amrit Sorli ,*Quantum Matter*,**2014** 3, 200-214
24. Monajjemi , M.; Honaparvar , B.; Khalili Hadad ,B.; Ilkhani ,AR.; Mollaamin, F.*Afr. J. Pharm. Pharmacol* .**2010**, 4 (8), 521-529
25. Björn Piglosiewicz, Jan Vogelsang.;Slawa Schmidt.; Doo Jae Park.; Petra Groß, .; Christoph Lienau ,*Quantum Matter,***2014** ,3, 297-306
26. Monajjemi, M. *Chemical Physics*. **2013,** *425*, 29-45
27. Fazaeli ,R.; Monajjemi ,M.; Ataherian ,F.; Zare, K. *Journal of Molecular Structure: THEOCHEM*.**2002**, *581 (1)*, 51-58
28. Monajjemi, M.; Mollaamin, F, *J Clust Sci*, 22(2011)673.
29. Medhat Ibrahim and Hanan Elhaes ,Rev. *Theor. Sci*. **2013**, *1,* 368-376
30. Anurag Srivastava.; Nileshi Saraf.; A. K. Nagawat , *Quantum Matter*,**2013,** *2*, 401-407
31. IIJIMA Sumio.; YUDASAKA Masako.; Nihey fumiyuki.; *NEC technical journal*,**2007,** *2*,1,
32. S. Iijima and T. Ichihasi, *Nature*,**1993**,*363*, 603

33. D. S. Bethune.;C. H. Kiang.; M. S. deVries.; G. Gorman, R. Savoy.; J. Vazques.; R. Beyers, *Nature* ,**1993**, *363*, 605
34. Monajjemi, M .; Aghaie , H.; Naderi , F. *Biochemistry (Moscow).***2007,** *72 (6)*, 652-657
35. Monajjemi, M*. Journal of Molecular Modeling* , **2014**, *20*, 2507
36. Davide Fiscaletti,Rev. *Theor. Sci*.**2013** 1, 103-144
37. Monajjemi , M.; Chahkandi ,B.; Zare,K.; Amiri, A. *Biochemistry (Moscow),***2005** *70 (3)*, 366-376
38. Monajjemi, M .; Afsharnezhad ,S.; Jaafari , M.R.; Abdolahi ,T.; Nikosade ,A.; Monajemi ,H.; *Russian Journal of physical chemistry A*, **2007,** *2*,1956-1963
39. Monajjemi, M.; Khaleghian, M, Journal of Cluster Science. **2011,** *22 (4)*, 673-692
40. Mollaamin , F.; Monajjemi , M , *Journal of Computational and Theoretical Nanoscience***. 2012**, *9 (4)* 597-601
41. Monajjemi, M. *Struct. Chem*, **2012**, *23* 551.
42. Mollaamin, F.; Gharibe, S.; Monajjemi, M. *Int. J. Phy. Sci* , **2011**,6, 1496-1500
43. Monajjemi, M .; Faham, R.; Mollaamin, F. *Fullerenes, Nanotubes, and Carbon Nanostructures* , **2012** *20*, 163–169
44. Monajjemi, M.; Khaleghian, M.; Tadayonpour, N.; Mollaamin, F. *International Journal of Nanoscience,* **2010**, 9 (05), 517-529
45. Mollaamin , F .; Najafi ,F.; Khaleghian, M.; Khalili Hadad, B.; Monajjemi ,M. *Fullerenes, Nanotubes, and Carbon Nanostructures*,**2011** *19*, 653–667
46. Monajjemi, M.; Chegini , H. ; Mollaamin , F. ; Farahani ,P, *Fullerenes, Nanotubes, and Carbon Nanostructures***.2011**,*19*, 469–482
47. Monajjemi, M.; Yamola ,H.; Mollaamin,F. *Fullerenes, Nanotubes, and Carbon Nanostructures*, **2014***, 22*, 595–603
48. Monajjemi, M.; Heshmata, M.; Haeri, HH , *Biochemistry (Moscow),***2006,** 71 (1), S113-S122
49. Xinjun Wang.; Yi Xie and Qixun Guo , *CHEM. COMMUN.* **2003**, 2688–2689
50. A. Rubio.; J.L. Corkill.; M.L. Cohen.; *Phys. Rev*. B ,**1994**, *49*, 5081
51. X. Blasé.; A. Rubio.; S.G. Louie.; M.L. Cohen.; *Europhys. Lett,* **1994**.*28*, 335.
52 . N.G. Chopra.; J. Luyken.; K. Cherry.; V.H. Crespi.; M.L. Cohen,S.G. Louie.; A. Zettl, *Science.***1995 ,** *269*, 966
53. N.G. Chopra.;A. Zettl.;*Solid State Commun*.**1998** ,*105*, 297
54. J. Cumings.; A. Zettl, *Solid State Commun*.**2004**, *129*, 661
55. R. Ma.; Y. Bando.; H. Zhu.; T. Sato, C. Xu, D. Wu, *J. Am.Chem. Soc*.**2002**, *124*, 7672,
56. P.W. Fowler, K.M. Rogers, G. Seifert, M. Terrones, and H. Terrones, *Chem. Phys*. Lett. **1999**, 299, 359
57. Monajjemi, M .; Falahati, M.; Mollaamin, F.; *Ionics,* **2013** , *19*, 155–164
58. Monajjemi , M.; Heshmat ,M.; Aghaei , H.; Ahmadi , R.; Zare,K. *Bulletin of the Chemical Society of Ethiopia,* **2007**, 21 (1)
59. Monajjemi , M.; Lee, V.S. ; Khaleghian, M.; B. Honarparvar, B.; F. Mollaamin, F, *J. Phys.Chem. C*. **2010**, *114 (2010)* 15315
60. A. Rubio, J.L. Corkill, M.L. Cohen, *Phys. Rev*. B.**1994**, 49,5081
61. X. Blase, A. Rubio, S.G. Louie, M.L. Cohen, *Europhys. Lett*. **1994**, 28 335.
62. N.G. Chopra, J. Luyken, K. Cherry, V.H. Crespi, M.L. Cohen,S.G. Louie, A. Zettl, *Science* ,**1995**, *269*, 966.
63. O.R. Lourie, C.R. Jones, B.M. Bartlett, P.C. Gibbons, R.S. Ruoff,W.E. Buhro, *Chem. Mater*.**2000**, *12* ,1808;
64. R. Ma, Y. Bando, T.Sato, *Chem. Phys. Lett*.**2001,** *337* ,61.
65. W. Han, Y. Bando.; K. Kurashima.; T. Sato, *Appl. Phys. Lett*.**1998,** *73*, 3085;
66. (a) D. Golberg.; Y. Bando.; M. Eremets.; K. Takemura.; K. Kurashima.;H.Yusa, *Appl. Phys. Lett*.**1996** ,*69,* 2045
67. D.P. Yu, X.S. Sun, C.S. Lee, I. Bello, S.T. Lee, H.D. Gu, K.M. Leung, G.W. Zhou, Z.F. Dong.; Z. Zhang.; *Appl. Phys. Lett*.**1998,** *72* , 1966.
68. F.Jensen.; H.Toftlund, *Chem. Phys. Lett*.**1993**, *201*,89 , 94
69. Monajjemi, M .; Sobhanmanesh, A .; Mollaamin, F. *Fullerenes, Nanotubes, and Carbon Nanostructures*,**2013**, *21* 47–63
70. Monajjemi ,M.; Karachi ,N.; Mollaamin, F. *Fullerenes, Nanotubes, and Carbon Nanostructures,* **,2014***,* 22: 643–662
71. Monajjemi, M.; Mahdavian, L.; Mollaamin, F.: *Bull .Chem.Soc.Ethiop* ,**2008**, *22(2),*1-10.
72. V. Tozzini.; F. Buda.; A. Fasolino.; *physical*

review letters ,**2000,***21,*85
73. G. Seifert.; P. W. Fowler.; Mitchell, D.; Porezag, D.; Frauenheim, Th. *Chem. Phys. Lett.* **1997**, *268*, 252
74. Mollaamin ,F.; Baei, MT.; Monajjemi, M.; Zhiani , R.; Honarparvar , B.; *Russian Journal of Physical Chemistry A*, *Focus on Chemistry,***2008**, 82 (13), 2354-2361
75. Monajjemi, M.; Ghiasi, R. ;Ketabi, S. *Journal of Chemical Research*.*2004*, 1: 11-18
76. Mahdavian,L.; Monajjemi, M.; Mangkorntong ,N.*Fullerenes, Nanotubes and Carbon Nanostructures*,2009, *17 (5)*, 484-495
77. Jon M. Matxain.; Jesus M. Ugalde.; M. D. Towler.; and R. J. Needs.; *J. Phys. Chem. A* **2003**, *107,* 10004-10010
78. WU Haishun.;XU Xiaohong,; JIAO Haijun, ZHANG Fuqiang .; JIA Jianfeng. *Chinese Science Bulletin.* **2003,** 48, 11 1102 1107
79. Monajjemi, M .; Ketabi ,S.; Amiri, A. *Russian Journal of Physical Chemistry* , **2006**, 80 (1), S55-S62
80. M. Monajjemi .; Robert Wayne Jr, J.E. Boggs, Chemical. Physics. 433 (2014) 1-11
81. Jon M. Matxain.; Jesus M. Ugalde.; M. D. Towler.; and R. J. Needs.; *J. Phys. Chem. A* **2003**, *107,* 10004-10010
82. WU Haishun.; XU iaohong.; JIAO Haijun, ZHANG Fuqiang .; JIA Jianfeng *Chinese Science Bulletin* **2003,** *48 (11),* 1102 1107
83. Monajjemi , M.; Honarparvar, B.; Monajemi, H.;. *Journal of the Mexican Chemical Society*, **2006**, 50 (4), 143-148
84. Monajjemi ,M.; Mollaamin ,F. *Journal of Computational and Theoretical Nanoscience*, **2012** ,*9 (12)* 2208-2214
85. Monajjemi, M.; Mahdavian, L.; Mollaamin, F.; Honarparvar, B. *Fullerenes, Nanotubes and Carbon Nanostructures*, **2010,** *18*, 45–55
86. Friedrich, B.; J.D. Weinstein.; R. Decarvalho .; J.M. Doyle.;. *Trap. J. Chem. Phys*. **1999,** *110*,2376-2383.
87. Ramsay, N.E.; Magnetic Shilding of Nuclei. *J. Phys. Rev*.**1950**, *78,* 699-703.
88. Frischend, M.J.; J.B. Foresman, **1995**. *Gaussian 94 user' reference (Gaussian, Inc., Pittsburgh).*
89. Ghalandari, B.; Monajjemi, M.; Mollaamin, F.; *Journal of Computational and Theoretical Nanoscience*, **2011** *8,* 1212–1219
90. Monajjemi , M.; Khosravi , M.; Honarparvar, B.; Mollaamin, F.; *International Journal of Quantum Chemistry***, 2011**, *111,* 2771–2777
91. Monajjemi, M.; Rajaeian, E.; Mollaamin, F. *Physics and Chemistry of Liquids*,**2008**, *46* 299.
92. Tahan, A .; Monajjemi, M. *Acta Biotheor,* **2011,** *59*, 291–312
93. Monajjemi, M.; Farahani, N.; Mollaamin, F. *Physics and Chemistry of Liquids*, **2012**, *50(2)* 161–172
94. Monajjemi, M.; Razavian, M.H.; Mollaamin,F.; Naderi,F.; Honarparvar,B.; *Russian Journal of Physical Chemistry A* , **2008** , *82 (13),* 2277-2285
95. Mollaamin , F.; Varmaghani , Z.; Monajjemi , M, Physics and Chemistry of Liquids. **2011**, *49* 318
96. Monajjemi, M.; Honarparvar, B.; H. Haeri, H.; Heshmat, M.; Russian Journal of *Physical Chemistry C*, **2008**, 80(1),S40-S44.
97. Cheeseman, J.R.; M.J. Frisch.; F.J. Devlin .;P.J.Stephens, *Chemical Physics Letters*, **1996**,*252 (3-4)*, 211-220.
98. Pisani, C.;S. Casassa .; P. Ugliengo, *Chemical Physics Letter*. **1996**, *253 (3-4)* 201-208.
99. Dresselhaus, M.; Dresselhaus, G.; Eklund, P. C., *Science of Fullerenes and Carbon Nanotubes, San Diego: Academic Press*, **1996**, *109*, 175.
100. Oku,T.; Nishiwaki ,A.; Narita,I.; Gonda,G.. *Chemical Physics Letters*, 2003, *380*, 620–623.
101. Nirmala,V.; Kolandaivel,P.; *Journal of Molecular Structure*, 2007, THEOCHEM, 817,137-145.
102. J.C. Charlier, J.C.; Rignanese,G.M. *Phys. Rev*. Lett, **2001**, 86, 5970.