



Adsorption of Si_6O_{12} on CNTs in View Point of NMR Shielding Tensors and NBO Analysis: A Novel Material for Drug Delivery

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ABSTRACT

The interaction of the Si_6O_{12} molecule over the CNTs have been investigated with density functional theory using HF and B3LYP method and 6-31G, 6-31G** and 6-311G** basis sets. We also analyze the electronic structure and charge Mulliken population for the energetically most favorable complexes. Our results indicate Si_6O_{12} can form stable bindings with CNTs via the Oxygen. The NMR shielding tensors have been investigated. The same Study performed for Si_7O_{14} and we found that this molecule can form stable bindings with CNTs via the Silicon site. Thus, we arrive at the prediction that the even number (Si_6O_6) has a different mechanism for adding to CNTs compare to add number such as Si_7O_{14} .

Key words:

INTRODUCTION

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 carbohydrates²⁸⁻³⁵.

The carbon nanotube (CNT) is a representative nano-material. CNT is a cylindrically

shaped carbon material with a nano-metric-level diameter¹⁻¹⁵.

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 seamlessly¹²⁻³⁰.

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 graphite²²⁻⁴².

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 released⁴²⁻⁵⁰.

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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 sheet⁷¹⁻⁸¹.

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

structure⁷⁹⁻⁹⁵. 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 single walled nanotubes were reported.

The carbon nanotube (CNT) is a representative nano-material. CNT is a cylindrically shaped carbon material with a nano-metric-level diameter⁹⁴⁻⁹⁸.

In the NBO analysis, the interaction arising from electron delocalization are analyzed by selecting a number of natural bonding and anti-bonding orbitals that distort from the idealized Lewis structure, caused by interactions among them through hyper-conjugative or electrostatic interactions. In NBO analysis, the input atomic orbital basis set is transformed via natural atomic orbitals (NAOs) and natural hybrid orbital (NHOs) into NBO. In the present theoretical study, particular attention has been paid to the structural properties of The Si6O12-CNTs and Si7O14-CNTs systems. So, the NBO analysis gives supplementary information of the relative structural properties. It should be noted that conjugated systems, such as benzene and p-conjugated linear molecules, have been well studied with NBO analysis.

Computational details

Calculations were performed using an all-electron linear combination of atomic orbitals Hatree-Fock (HF) and density functional theory (DFT) calculations using the Gaussian 03 package.

Table 1:

Nucleus list:			
1(C)	>-->	Charge: 0.000000	x, y, z (Bohr): -3.678102 1.693832 2.220798
2(C)	>-->	Charge: 0.000000	x, y, z (Bohr): -3.734370 -1.701905 -2.210497
3(C)	>-->	Charge: 0.000000	x, y, z (Bohr): -4.594693 2.624239 -1.691881
4(C)	>-->	Charge: 0.000000	x, y, z (Bohr): -4.552326 -2.621177 1.731134
5(C)	>-->	Charge: 0.000000	x, y, z (Bohr): -0.001473 1.974335 -1.553599
6(C)	>-->	Charge: 0.000000	x, y, z (Bohr): -0.003967 5.554373 0.527634
7(C)	>-->	Charge: 0.000000	x, y, z (Bohr): 0.002430 -1.962876 1.487237
8(C)	>-->	Charge: 0.000000	x, y, z (Bohr): 0.003767 -5.545408 -0.559926
9(Si)	>-->	Charge: 1.000000	x, y, z (Bohr): -5.127190 -0.001755 0.025180
10(Si)	>-->	Charge: 1.000000	x, y, z (Bohr): -2.222398 3.409768 0.105590
11(Si)	>-->	Charge: 1.000000	x, y, z (Bohr): -2.232685 -3.121486 -0.130889
12(Si)	>-->	Charge: 1.000000	x, y, z (Bohr): 2.216083 3.410901 0.108908
13(C)	>-->	Charge: 0.000000	x, y, z (Bohr): 1.593568 2.634073 -1.685559
14(C)	>-->	Charge: 0.000000	x, y, z (Bohr): 3.670742 1.691072 2.222343
15(C)	>-->	Charge: 0.000000	x, y, z (Bohr): 1.561316 -2.620867 1.721309
16(C)	>-->	Charge: 0.000000	x, y, z (Bohr): 3.733193 -1.691851 -2.212693
17(Si)	>-->	Charge: 1.000000	x, y, z (Bohr): 2.237694 3.119404 0.133405
18(Si)	>-->	Charge: 1.000000	x, y, z (Bohr): 5.428448 0.000000 0.000000
Note: Orbital 50 is HOMO, energy: 0.219253 a.u. 5.966165 eV			
Orbital 61 is LUMO, energy: -0.214073 a.u. -5.825228 eV			
LUMO/HOMO gap: 0.005179 a.u. 0.140939 eV 13.599593 kJ/mol			

Table 2: NMR parameters of Silicon and Oxygen in Si₆O₁₂CNTs and Si₇O₁₄CNTs at the different levels

	δ	η	σ_{aniso}	σ_{iso}	Atom
B3LYP/6-311G** Si6O12CNTs	(1)O	129	49.5	-18.9	0.25
	(2)O	65.1	81	-45	0.8
	(3)O	50.4	92.7	-51.5	0.79
	(4)O	-26.7	277.6	-133.2	0.61
	(5)O	58.3	57.2	-22.8	0.3
	(6)O	177	120.3	-59	0.64
	(7)O	76.9	324	-159.8	0.64
	O(8)	108.6	53.3	-20	0.22
	O(9)	159.1	21.9	-13	0.87
	O(10)	47.2	92.1	-54.8	0.88
	O(11)	171.8	35.9	-18.8	0.72
	O(12)	203.8	45	-55.1	0.08
	Si(1)	179.4	16.5	-16.2	0.35
	Si(2)	183	16.3	-9.4	0.84
	Si(3)	159.3	26.9	-24.2	0.48
	Si(4)	72.3	74.4	-42.2	0.82
Si(5)	164.6	49.8	-19.3	0.28	
Si(6)	167	48.8	-18.1	0.2	
B3LYP/6-31G Si6O12CNTs	(1)O	175.5	33.7	-19.3	0.83
	(2)O	90	317.1	-159.6	0.67
	(3)O	79.1	80.5	-43.4	0.76
	(4)O	20.8	255.5	-129.4	0.68
	(5)O	94.2	46.03	-19.2	0.4
	(6)O	217.8	126.5	-56.6	0.5
	(7)O	75.7	81.9	-56	0.94
	O(8)	203.5	52.2	-62.04	0.12
	O(9)	187.5	16.9	-9.4	0.8
	O(10)	74.6	76.2	-45.6	0.8
	O(11)	131	83.3	-72.7	0.52
	O(12)	179.5	37.2	-20	0.76
	Si(1)	200.3	14.1	-15.1	0.23
	Si(2)	207.4	131.7	-58	0.48
	Si(3)	185.8	20.4	-20.3	0.34
	Si(4)	77.8	67.8	-42.5	0.93
Si(5)	160.7	88.5	-65.5	0.8	
Si(6)	142	56.1	-24	0.4	
B3LYP/6-311G** Si7O14CNTs	(1)O	90.5	44.7	-30.9	0.92
	(2)O	97	308.8	152.4	0.64
	(3)O	75.4	77.1	-41.2	0.75
	(4)O	93.9	46.3	-33.2	0.85
	(5)O	95.7	45.6	-19.2	0.42
	(6)O	220.2	117.5	-53.4	0.53
	(7)O	73	80.1	-51.1	0.95
	O(8)	83.3	48.4	-34.3	0.87
	O(9)	139.9	42.6	-23.1	0.77

	O(10)	49.9	92.7	-57.1	0.91
	O(11)	162.3	53.1	-59.4	0.19
	O(12)	65.1	81	-45.1	0.8
	O(13)	55.6	-45.6	101.5	0.51
	O(14)	155.3	-19.6	44.8	0.47
	Si(1)	196.3	12.7	-13	0.3
	Si(2)	165.2	35.3	-18.2	0.7
	Si(3)	183.5	21.1	-19.4	0.44
	Si(4)	75.9	65.4	-39.5	0.89
	Si(5)	176.7	77.9	-60.5	0.71
	Si(6)	138.3	48.5	-18.6	0.26
	Si(7)	98.4296	75.4	-88.8	0.13
B3LYP/6-31G Si7O14CNTs	(1)O	135.1	55	-23.6	-0.44
	(2)O	32.5	256.6	-128.7	-0.67
	(3)O	67.6	81.7	-43.2	-0.73
	(4)O	8.15	269.41	-137.3	-0.69
	(5)O	86.57	51.01	-20.6	-0.35
	(6)O	156.8	39.8	-22.5	-0.82
	(7)O	65.2	85	-54.1	-0.95
	O(8)	190.53	46.7	-58.5	0.06
	O(9)	174	18.4	-10.2	-0.8
	O(10)	55	79.8	-45.26	-0.82
	O(11)	156	51.5	-19.78	-0.26
	O(12)	167.8563	35.8143	-20.5798	-0.83
	O(13)	187.6	95.83	-41.2	0.45
	O(14)	29.1	115.6	-70.7	0.9
	Si(1)	188.9	15.2	-14.5	0.39
	Si(2)	156.6	35.9	-18.6	-0.71
	Si(3)	175.7	23.6	-21.2	0.48
	Si(4)	68.8	71.3	-42.8	-0.89
	Si(5)	162.2	87.43	-67.24	0.73
	Si(6)	129	49.5	-18.9	-0.25
	Si(7)	41.287	70.4	-41.3	0.86

The optimizations of antibiotics and Si₆O₁₂ are carried out including exchange and correlation contributions using Beck's three parameter hybrid and Lee-Yang-Parr (LYP) correlation [B3LYP]; including both local and non local terms. We have geometric optimization calculation at the HF/6-31G, HF/6-31G**, HF/6-311G**. We have also performed a geometric optimization calculation at the B3LYP/6-31G, B3LYP/6-31G** and B3LYP/6-31G** level.

The NMR isotropic shielding constants were calculated using the standard GIAO (Gauge-Independent Atomic Orbital) approach of Gaussian 03 program package.

a) The isotropic value σ_{iso} of the shielding tensor which can be defined as:

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

b) The anisotropy parameter ($\Delta\sigma$) defined as:

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

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

and

c) The asymmetry parameter (ζ) which is given by:

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

Table 3: Summary of Natural Population Analysis

Natural	Atom No	Charge	Core	Valence	Rydberg	Total
O	1	-1.03191	1.99983	7.02846	0.00362	9.03191
O	2	-1.03280	1.99983	7.02937	0.00360	9.03280
O	3	-0.99952	1.99982	6.99622	0.00348	8.99952
O	4	-0.99456	1.99982	6.99123	0.00351	8.99456
O	5	-1.09586	1.99983	7.09217	0.00386	9.09586
O	6	-1.06143	1.99980	7.05852	0.00311	9.06143
O	7	-1.09858	1.99982	7.09490	0.00386	9.09858
O	8	-1.06326	1.99980	7.06038	0.00308	9.06326
Si	9	1.95810	10.00000	2.00789	0.03401	12.04190
Si	10	2.12946	10.00000	1.83252	0.03801	11.87054
Si	11	2.13076	10.00000	1.83150	0.03774	11.86924
Si	12	2.12971	10.00000	1.83228	0.03801	11.87029
O	13	-1.00017	1.99982	6.99687	0.00348	9.00017
O	14	-1.03137	1.99983	7.02792	0.00362	9.03137
O	15	-0.99548	1.99982	6.99215	0.00351	8.99548
O	16	-1.03226	1.99983	7.02883	0.00360	9.03226
Si	17	2.13094	10.00000	1.83132	0.03774	11.86906
Si	18	1.95821	10.00000	2.00777	0.03402	12.04179
* Total *		0.00000	83.99786	95.74030	0.26185	180.00000

Table 4: Natural Electron Configuration

Atom No	valance/core	
O	1	[core]2S(1.80)2p(5.23)
O	2	[core]2S(1.80)2p(5.23)
O	3	[core]2S(1.79)2p(5.20)
O	4	[core]2S(1.79)2p(5.20)
O	5	[core]2S(1.80)2p(5.29)
O	6	[core]2S(1.78)2p(5.28)
O	7	[core]2S(1.80)2p(5.30)
O	8	[core]2S(1.77)2p(5.29)
Si	9	[core]3S(0.79)3p(1.21)4p(0.03)
Si	10	[core]3S(0.62)3p(1.21)4S(0.01)4p(0.03)
Si	11	[core]3S(0.62)3p(1.21)4S(0.01)4p(0.03)
Si	12	[core]3S(0.62)3p(1.21)4S(0.01)4p(0.03)
O	13	[core]2S(1.79)2p(5.21)
O	14	[core]2S(1.80)2p(5.23)
O	15	[core]2S(1.79)2p(5.20)
O	16	[core]2S(1.80)2p(5.23)
Si	17	[core]3S(0.62)3p(1.21)4S(0.01)4p(0.03)
Si	18	[core]3S(0.79)3p(1.21)4p(0.03)

RESULTS AND DISCUSSION

We studied about Si_6O_{12} and Si_7O_{14} molecules as the novel material for drug delivery.

Before and after connecting to the CNTs. NMR and NBO calculations were performed in electric field of charges. NMR and NBO parameters are listed in tables 1-5 in different levels and different basis sets.

HOMO and LUMO and Gap energy of MWC-Nano-cones are listed in Table1.

Contour line map of Localized orbital Locator (LOL) and Relief map (Shaded Surface map with projection) for electron density of Si_6O_{12} are shown in Fig2&3. electron Localization Function of Si_6O_{12} is shown in Fig 4.

The situation of Si_6O_{12} adsorption over

Table 5: Natural bond orbital analysis

Occupancies	Lewis Structure				Low High		(NL)	Dev	
	Thresh	Lewis	Non-Lewis	CR BD 3C LP (L)	occ	occ			
Cycle									
1(1)	1.90	174.53005	5.46995	12 27 0 21	19	27	0.13		
2(2)	1.90	174.53151	5.46849	12 27 0 21	19	27	0.13		
3(3)	1.90	174.53151	5.46849	12 27 0 21	19	27	0.13		
4(1)	1.80	174.65362	5.34638	12 27 0 21	1	27	0.71		
5(2)	1.80	174.72293	5.27707	12 28 0 20	0	28	0.13		
6(3)	1.80	174.72293	5.27707	12 28 0 20	0	28	0.13		
7(1)	1.70	171.93387	8.06613	12 16 0 32	1	24	0.73		
8(2)	1.70	172.06530	7.93470	12 16 0 32	1	24	0.73		
9(3)	1.70	171.87814	8.12186	12 16 0 32	3	25	0.71		
10(4)	1.70	171.93387	8.06613	12 16 0 32	1	24	0.73		
11(5)	1.70	172.06530	7.93470	12 16 0 32	1	24	0.73		
12(6)	1.70	171.87814	8.12186	12 16 0 32	3	25	0.71		
13(7)	1.70	171.93387	8.06613	12 16 0 32	1	24	0.73		
14(8)	1.70	172.06530	7.93470	12 16 0 32	1	24	0.73		
15(9)	1.70	171.87814	8.12186	12 16 0 32	3	25	0.71		
16(1)	1.60	169.38902	10.61098	12 4 0 44	0	24	0.73		
17(2)	1.60	169.22759	10.77241	12 4 0 44	0	24	0.73		
18(3)	1.60	169.22759	10.77241	12 4 0 44	0	24	0.73		
19(4)	1.60	169.22759	10.77241	12 4 0 44	0	24	0.73		
20(5)	1.60	169.22759	10.77241	12 4 0 44	0	24	0.73		
21(6)	1.60	169.22759	10.77241	12 4 0 44	0	24	0.73		
22(7)	1.60	169.22759	10.77241	12 4 0 44	0	24	0.73		
23(8)	1.60	169.22759	10.77241	12 4 0 44	0	24	0.73		
24(9)	1.60	169.22759	10.77241	12 4 0 44	0	24	0.73		
25(1)	1.50	168.41325	11.58675	12 0 0 48	0	24	0.73		
26(2)	1.50	168.41325	11.58675	12 0 0 48	0	24	0.73		
27(1)	1.80	174.72293	5.27707	12 28 0 20	0	28	0.13		

Structure accepted: RESONANCE keyword permits strongly delocalized structure

Effective Core	60.00000	Core	23.99785 (99.991% of 24)
Valence Lewis	90.72508 (94.505% of 96)	Total Lewis	174.72293 (97.068% of 180)
Valence non-Lewis	5.04717 (2.804% of 180)	Rydberg non-Lewis	0.22990 (0.128% of 180)
Total non-Lewis	5.27707 (2.932% of 180)		

Table 6: Natural Bond Orbitals Summary

Principal	Delocalization	NBO	Occupancy	Energy geminal, vicinal, remote
1. BD (1) O	1 -Si 9	1.87941	-0.56226	163(g),167(g),165(g),96(g)
2. BD (1) O	1 -Si 10	1.92550	-0.64049	161(g),166(g),171(g),105(g)
3. BD (2) O	1 -Si 10	1.82990	-0.34040	169(g),161(g),171(g),105(g)
4. BD (1) O	2 -Si 9	1.90043	-0.61423	167(g),163(g),165(g),96(g)
5. BD (2) O	2 -Si 9	1.83917	-0.30943	167(g),165(g),173(v),96(g)
6. BD (1) O	2 -Si 11	1.94562	-0.70204	173(g),168(g),95(v),167(v)
7. BD (1) O	3 -Si 9	1.86082	-0.45296	159(g),162(g),167(g),163(g)
8. BD (1) O	3 -Si 10	1.92039	-0.68742	169(g),161(g),105(g),160(g)
9. BD (1) O	4 -Si 9	1.80147	-0.39265	159(g),163(g),165(g),162(g)
10. BD (1) O	4 -Si 11	1.95367	-0.71006	173(g),164(g),165(v),162(v)
12. BD (1) O	5 -Si 12	1.86911	-0.57783	179(g),172(g),177(g),122(g)
13. BD (1) O	6 -Si 10	1.89379	-0.66554	169(g),161(g),121(v),160(g)
14. BD (1) O	6 -Si 12	1.89334	-0.66492	170(g),179(g),104(v),122(g)
15. BD (1) O	7 -Si 11	1.93844	-0.66897	176(v),182(v),185(v),145(v)
16. BD (1) O	7 -Si 17	1.86963	-0.58112	185(g),176(g),182(g),146(g)
17. BD (1) O	8 -Si 11	1.92651	-0.72737	182(v),173(g),174(v),164(g)
18. BD (1) O	8 -Si 17	1.89564	-0.67064	174(g),185(g),113(v),184(g)
19. BD (1)Si	12 - O 13	1.92045	-0.68885	170(g),179(g),122(g),178(g)

CNTs and The situation of Si_7O_{14} are shown in Fig1. 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 , $\Delta\delta$ and η for this nano-cone in the same methods and basis sets are shown in table 2. Finally the charts of σ_{iso} , σ_{aniso} , σ and η for the atoms of Si_6O_{12} , Si_7O_{14} in 6-31G, 6-

311G**, level of theory and B3LYP method. We can obtain the interesting results from the NMR charts. Comparison of these charts (σ_{iso} , σ_{aniso} , σ 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

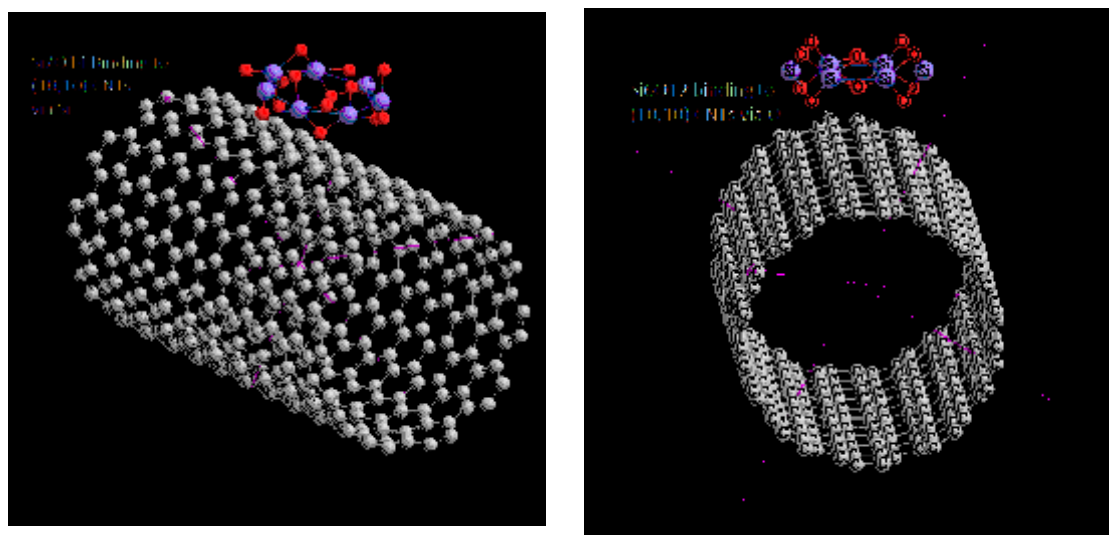


Fig. 1: Si_6O_{12} & Si_7O_{14} binding to (10,10)CNTs in different direction a) via Oxygen b) Via Silicone

are exactly repeated in σ_{iso} , σ_{aniso} , σ and η charts. These three atoms are the active sites in these structures. In general, the chart of electronic charge in different methods and basis sets is similar to the charts of NMR parameters Silicon atoms have more electrons than oxygen atoms.

So we can find that most chemical shielding. The concavity points are created due to the change of negative charge into a positive charge.

The electron density figure show that the mechanism of positive charge is different from

negative charge. Positive and negative areas are completely different.

The results show that the heterocycle drugs connect to Si_6O_{12} is stronger than Si_7O_{14} .

NBO analysis of the Si_6O_{12} and Si_7O_{14} system at the level of B3LYP/6-31g theory with different has been given in Table 3-6. The coefficients of s and p orbitals of both Si-O in Si_6O_{12} and Si_7O_{14} bonds can be distinguished based on these NBO data. Based on the constant values of the coefficients of linear combination of s and p orbitals of different bonds, a specific voltage differences could be

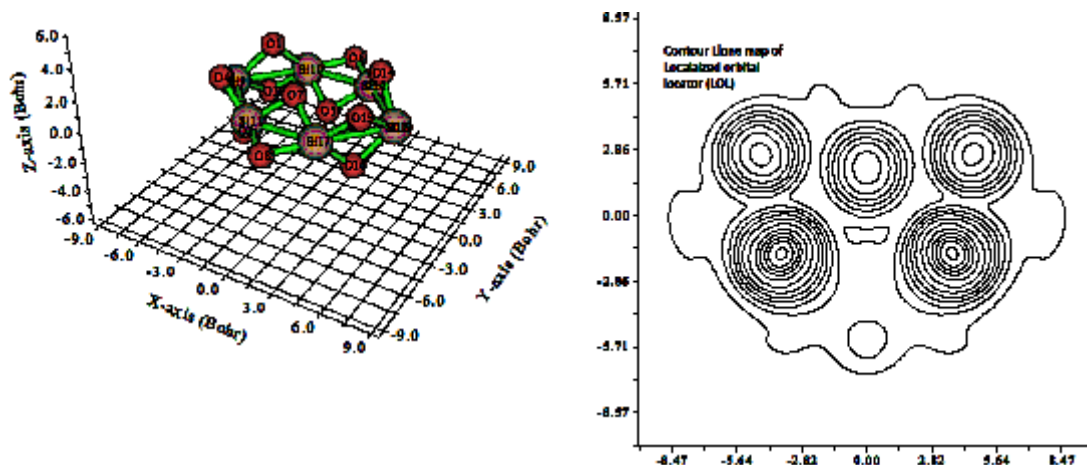


Fig. 2: Contour line map of Localized orbital Locator (LOL)

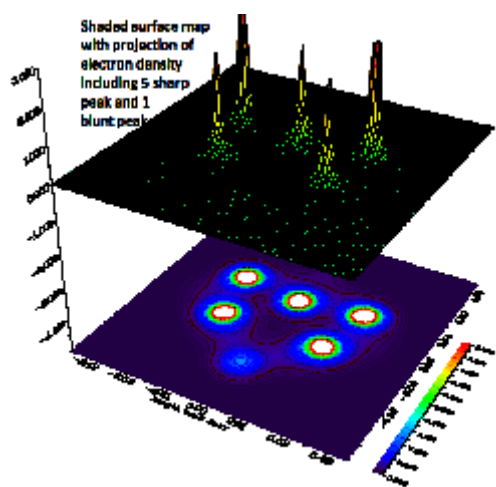


Fig. 3: Shaded Surface map with projection of electron density including 5 sharp peak and one blunt

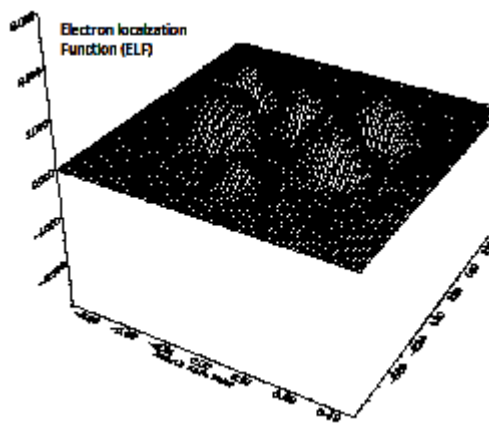


Fig. 4: Electron Localization Function of Si_6O_{12}

expected. Summary of Natural Population analysis and Natural Population is listed in Table 3. Natural electron configuration of Valance and core electrons

is listed in table 4. Occupancy, geminal, vicinal, energy, NBO, Principal delocalization is listed in Table 6.

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