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 carbohydrates.28-35

The carbon nanotube (CNT) is a representative nano-material. CNT is a cylindrically shaped carbon material with a nano-metric-level diameter.1-15. 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 seamlessly.12-30

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 graphite.22-42

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 released.42-50

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 nanometers50-63.

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.60-74

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.71-81

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 structure79-99. 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 diameter.94-98

In the NBO analysis, the interaction arising from electron delocalization are analyzed by selecting a number of natural bonding and antibonding 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.

### Computacional details

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

### Table 1:

| Nucleus List | Charge | x, y, z (Bohr) | Energy (a.u.) |
|-------------|--------|---------------|---------------|
| CO          | 8.00000 | x, y, z (Bohr) | -3.678102     |
| CO          | 8.00000 | x, y, z (Bohr) | -3.734370     |
| CO          | 8.00000 | x, y, z (Bohr) | -3.548378     |
| CO          | 8.00000 | x, y, z (Bohr) | -3.523262     |
| CO          | 8.00000 | x, y, z (Bohr) | -3.553535     |
| CO          | 8.00000 | x, y, z (Bohr) | -3.553535     |
| CO          | 8.00000 | x, y, z (Bohr) | -3.553535     |
| CO          | 8.00000 | x, y, z (Bohr) | -3.553535     |
| CO          | 8.00000 | x, y, z (Bohr) | -3.553535     |

| LUMO-LUMO gap | 0.005179 a.u. | 0.110229 eV |
|---------------|--------------|-------------|
| LUMO-HOMO gap | 13.595330 kJ/mol |
Table 2: NMR parameters of Silicon and Oxygen in Si₆O₁₂CNTs and Si₇O₁₄CNTs at the different levels

| Atom       | δ    | η   | σ_{aniso} | σ_{iso} | Atom |
|------------|------|-----|-----------|---------|------|
| B3LYP/6-31G** Si₆O₁₂CNTs | O(1) | 129 | 49.5 | -18.9 | 0.25 |
|           | O(2) | 65.1 | 81 | -45 | 0.8 |
|           | O(3) | 50.4 | 92.7 | -51.5 | 0.79 |
|           | O(4) | -26.7 | 277.6 | -133.2 | 0.61 |
|           | O(5) | 58.3 | 57.2 | -22.8 | 0.3 |
|           | O(6) | 177 | 120.3 | -59 | 0.64 |
|           | O(7) | 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 | O(1) | 175.5 | 33.7 | -19.3 | 0.83 |
|           | O(2) | 90 | 317.1 | -159.6 | 0.67 |
|           | O(3) | 79.1 | 80.5 | -43.4 | 0.76 |
|           | O(4) | 20.8 | 255.5 | -129.4 | 0.68 |
|           | O(5) | 94.2 | 46.03 | -19.2 | 0.4 |
|           | O(6) | 217.8 | 126.5 | -56.6 | 0.5 |
|           | O(7) | 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 | O(1) | 90.5 | 44.7 | -30.9 | 0.92 |
|           | O(2) | 97 | 308.8 | 152.4 | 0.64 |
|           | O(3) | 75.4 | 77.1 | -41.2 | 0.75 |
|           | O(4) | 93.9 | 46.3 | -33.2 | 0.85 |
|           | O(5) | 95.7 | 45.6 | -19.2 | 0.42 |
|           | O(6) | 220.2 | 117.5 | -53.4 | 0.53 |
|           | O(7) | 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 |
The optimizations of antibiotics and Si$_6$O$_{12}$ are carried out including exchange and correlation contributions using Becke’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.

|            | B3LYP/6-31G                      | Si7O14CNTs                    |
|------------|---------------------------------|------------------------------|
| 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        |                              |
| (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)      | 41.28770.4 -41.3 0.86         |                              |

a) The isotropic value $\sigma_{iso}$ 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:

$$\Delta\sigma = \sigma_{11} - \frac{\sigma_{22} + \sigma_{33}}{2}$$

If $|\sigma_{11} - \sigma_{iso}| \geq |\sigma_{33} - \sigma_{iso}|$ 

If $|\sigma_{11} - \sigma_{iso}| \leq |\sigma_{33} - \sigma_{iso}|$

and

c) The asymmetry parameter ($\zeta$) which is given by:
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    | 7.02792     | 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    | 6.96687     | 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) |
| Si 13   | [core]2S( 1.79)2p( 5.21)     |
| Si 14   | [core]2S( 1.80)2p( 5.23)     |
| Si 15   | [core]2S( 1.79)2p( 5.20)     |
| Si 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\textsubscript{6}O\textsubscript{12} and Si\textsubscript{7}O\textsubscript{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.

Table 5: Natural bond orbital analysis

| Occupancies | Lewis Structure | Low | High |
|-------------|-----------------|-----|------|
| Cycle       | Occ.            |     |      |
| 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)       | 1.70 171.93387 8.06613 | 12 16 0 32 | 3 25 | 0.71 |
| 13(7)       | 1.70 171.87814 8.12186 | 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)       | 1.70 171.93387 8.06613 | 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) |
| 11. BD (1) O | 5 - Si 12 | 1.86911 | -0.57783 | 179(g), 172(g), 177(g), 122(g) |
| 12. BD (1) O | 6 - Si 10 | 1.89379 | -0.66554 | 169(g), 161(g), 121(v), 160(g) |
| 13. BD (1) O | 6 - Si 12 | 1.89334 | -0.66492 | 170(g), 179(g), 104(v), 122(g) |
| 14. BD (1) O | 7 - Si 11 | 1.93844 | -0.66897 | 176(v), 182(v), 185(v), 145(v) |
| 15. BD (1) O | 7 - Si 17 | 1.86963 | -0.58112 | 185(g), 176(g), 182(g), 146(v) |
| 16. BD (1) O | 8 - Si 11 | 1.92651 | -0.72737 | 182(v), 173(g), 174(v), 164(g) |
| 17. BD (1) O | 8 - Si 17 | 1.89564 | -0.67064 | 174(g), 185(g), 113(v), 184(g) |
| 18. BD (1) O | 12 - O 13 | 1.92045 | -0.68885 | 170(g), 179(g), 122(g), 178(g) |

Fig. 1: Si6O12 & Si7O14 binding to (10,10)CNTs in different direction a) via Oxygen b) Via Silicone
are exactly repeated in $\sigma_{iso}$, $\sigma_{aniso}$, $\sigma$ and $\eta$ 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 $\text{Si}_6\text{O}_{12}$ is stronger than $\text{Si}_7\text{O}_{14}$.

NBO analysis of the $\text{Si6O12}$ and $\text{Si7O14}$ 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 $\text{Si6O12}$ and $\text{Si7O14}$ 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
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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