



## QM/MM & Monte Carlo Simulation of Single Wall Nano tube Carbon SWNT (15, 15) Binding Withthymine Dimer

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### ABSTRACT

In this research, we have studied of thymine dimer binding on the relative energies and dipole moment values and the structural properties of solvent effect (water, methanol and ethanol) surrounding single-walled and multi walled carbon nanotube, by using QM/MM simulation, those calculations have carried out with the Gaussian and Hyper Chem package. In this study we investigated the polar solvents effects on SWCNT within the Onsager self - consistent reaction field (SCRF) model using a Hartree-Fock method and the temperature effect on the stability of SWCNT in various. Because some of the Physicochemical parameters related to structural properties of SWCNT, we used different force fields to determine energy and other types of geometrical parameters, on the particular SWCNT, Because of the differences among force fields, the energy of a molecule calculated using two different force fields will not be the same. It is important to understand the energetic, stability dependent physical properties of armchair (m, n) carbon nanotube. In this study, the difference in force fields illustrated by comparing the calculated energies by using force fields such as AMBER ,MM+, and BIO+ .The quantum Mechanics calculations were carried out with the GAUSSIAN 98 program based on density functional theory (DFT) at the B1LYP/6-31G\* level. Normal Mode Analysis is an important tool for studying the structure and dynamics of Nano-sized systems. The vibrational frequencies obtained can be used to relate observed spectra to the details of the molecular structure, dynamics and other thermodynamic properties.

**Key words:** SWCNT,DFT,Thymine Dimer, NMR

### INTRODUCTION

The carbon nanotube (CNT) is a representative nano-material. CNT is a cylindrically shaped carbon material with a nanometric-level diameter<sup>1-8</sup>.

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<sup>9-15</sup>.

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<sup>16, 17</sup>.

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<sup>18,19</sup>.

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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<sup>21-23</sup>.

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<sup>24</sup>. The first report by Iijima was on the multiwall form, coaxial carbon cylinders with a few tens of nanometers in outer diameter<sup>25</sup>. Two years later single walled nanotubes were reported<sup>26,27</sup>. SWCNTs have considered as the leading candidate for nanodevice applications because of their one-dimensional electronic band 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<sup>28-35</sup>.

So, The structure of SWCNT as well as their dipole moments and relative energies have been studied by molecular dynamics simulation and quantum mechanics calculations within the Onsager self-consistent reaction field (SCRf) model using a Hartree-Fock method (HF) at the BLYP/6-21G\* level and the structural stability of considered nanotube in different solvent media and temperature have been compared and analyzed. We investigate effects of water, methanol and a mixture of them on

interaction of Thymine-dimer with SWCNT, utilizing these force fields too<sup>36-40</sup>.

The interaction of Thymine-Dimer with open-end of SWCNT in gas phase, water and methanol have been processed applying the abinitio calculations.

The calculations have been done with the GAUSSIAN 98 program according to DFT theory at the HF/6-31g\* level. Gibbs free energy, enthalpy, entropy and dipole moment values are compared in gas phase, water and methanol, in this research<sup>41</sup>. Thus, by utilizing a Hartree-Fock method, we studied the effects of different solvents on interaction of Thymine-dimer with open-end of SWCNT within the Onsager self-consistent reaction field (SCRf) model, and the temperature effects on the stability of the interaction between Thymine-dimer and single-walled carbon in various solvents<sup>42-44</sup>.

## Theoretical Background

### A Normal mode

A harmonic oscillator approximation is most widely used for computing molecular vibrational frequencies because more accurate methods require very large amounts of CPU time. Frequencies computed with the Hartree-Fock approximation and a quantum harmonic oscillator approximation tends to be 10% too high due to the harmonic oscillator approximation and lack of electron correlation<sup>45-47</sup>.

Many studies have shown that the carbon nanotubes possess remarkable mechanical and physical properties leading to many potential applications such as fluid transport, fluid storage at nanoscale, and nano-devices for drug delivery. Since controlled experiments at the nanometer scale are very difficult, the simulation techniques have been widely and successfully used to investigate the mechanical property, wave propagation and resonant frequency<sup>48</sup>.

The vibration of molecules is best described using a quantum mechanical approach. A harmonic oscillator does not exactly describe molecular vibrations. Bond stretching is better described by a Morse potential and conformational changes have sine-wave-type behavior. However,

the harmonic oscillator description is very useful as an approximate treatment for low vibrational quantum numbers<sup>49-55</sup>.

#### DFT Concept and Monte Carlo simulation

Because of imperfections of the force field, this lowest energy basin usually does not correspond to the native state in most cases, so the rank of native structure in those decoys produced by the force field itself is poor.

In density function theory the exact exchange for a single determination is replaced by a more general expression the exchange correlation functional, which can include terms accounting for both exchange energy and the electron correlation, which is omitted from Hartree-Fock theory:

$$E_{ks} = \nu + \langle hp \rangle + 1/2 \langle P_j(\rho) \rangle + E_{x(\rho)} + E_{c(\rho)}$$

Where  $E_{x(\rho)}$  is the exchange function and  $E_{c(\rho)}$  is the correlation functional.

The Metropolis implementation of the Monte Carlo algorithm has been developed by studying the equilibrium thermodynamics of many-body systems. Choosing small trial moves, the trajectories obtained applying this algorithm agree with those obtained by Langevin's dynamics<sup>59</sup>. This is understandable because the Monte Carlo simulations always detect the so-called "important phase space" regions which are of low energy<sup>60</sup>.

The correlation function of Lee, Yang and Parr includes both local and non-local term<sup>61-64</sup>.

#### Simulation of Langevin dynamics

The Langevin equation is a stochastic differential equation in which two force terms have been added to Newton's second law to approximate the effects of neglected degrees of freedom<sup>65</sup>. These simulations can be much faster than molecular dynamics. The molecular dynamics method is useful for calculating the time dependent properties of an isolated molecule. However, more often, one is interested in the properties of a molecule that is interacting with other molecules<sup>66</sup>.

#### Calculation details

In general, the electron distribution around a nucleus in a molecule is more spherically symmetric. Therefore, the size of electron current around the field, and hence the size of the shielding, will depend on the orientation of the molecule within the applied field  $B_0$ .

For chemical shielding (CS) tensor which describes how the size of shielding varies with molecular orientation?

The term "Ab Initio" is given to computations which are derived directly from theoretical principles, with no inclusion of experimental data. The most common type of ab initio calculation is called a Hartree Fock calculation (abbreviated HF), in which the primary approximation is called the central field approximation. A method, which avoids making the HF mistakes in the first place, is called Quantum Monte Carlo (QMC). There are several flavors of QMC variational, diffusion and Green's functions. These methods work with an explicitly correlated wave function and evaluate integrals numerically using a Monte Carlo integration. These calculations can be very time consuming, but they are probably the most accurate methods known today. In general, ab initio calculations give very good qualitative results and can give increasingly accurate quantitative results as the molecules in question become smaller<sup>67</sup>.

There are three steps in carrying out any quantum mechanical calculation in HyperChem 7.0 program package<sup>68</sup>. First, prepare a molecule with an appropriate starting geometry. Second, choose a calculation method and its associated options. Third, choose the type of calculation with the relevant options.

DFT is based on a theorem due to Hohenberg and Kohn, which states that all ground state properties are functions of the total electronic charge density  $\chi(r)$ . There are several different DFT functionals available differing primarily in the choice of the basis set functions, in which, the electronic wave functions are expanded and the scheme of integration<sup>69,70</sup>.

The Becke's three parameter exact exchange functional (B3) combined with gradient corrected correlation functional of Lee–Yang–Parr (LYP) have been employed to calculate energy, dipole moment, charge distribution and thermochemical data and NMR parameters by implementing the 6-31G,STO-3G basis sets. All the NMR shielding parameters were calculated supposing gauge-included atomic orbital (GIAO) method.

NMR spectroscopy is a research technique that exploits the magnetic properties of certain atomic nuclei to determine physical and chemical properties of atoms or the molecules in which they are contained. It relies on the phenomenon of nuclear magnetic resonance and

can provide detailed information about the structure, dynamics, reaction state, and chemical environment of molecules. Ab initio calculation of nuclear magnetic shielding has become an indispensable aid in the analysis of molecular structure and accurate assignment of NMR spectra of compounds.

NMR is based on the quantum mechanical property of nuclei. The chemical shielding refers to the phenomenon, which is 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.

Calculations of nucleus-dependent and -independent chemical shifts were carried out using the gauge-invariant atomic orbital (GIAO) approach.

**Table 1 : Thymine dimer simulation data**

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NAtoms=395 NActive=395 NUniq= 395 SFac= 7.50D-01 NATfMM=80 NAOKFM=T Big=T  
 UHF-Huckel (Hoffmann) calculation of energy.  
 MO and density RWFs will be updated.  
 MinBas: lTypMB=3 Store=F.  
 MinBas: lTypMB=3 Store=T.  
 Entering OneEill...  
 Overlap between basis sets.  
 Requested accuracy = 0.1000D-12  
 PrsmSu: NPrtUS=1 ThrOK=F lAlg=1  
 PRISM was handed 14567655 working-precision words and 134310 shell-pairs  
 lPart= 0 NShTot= 134310 NBatch= 183 AvBlEn= 733.9  
 CnvPC2: ToCart=F DoDens=F lPureD=0 lPureF=0.

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Huckel eigenvalues -	-1.323	-1.311	-1.310	-1.310	-1.310	-1.310	-1.309	-1.309	-1.309	-1.308
Huckel eigenvalues -	-1.308	-1.308	-1.307	-1.307	-1.306	-1.306	-1.306	-1.306	-1.298	-1.296
Huckel eigenvalues -	-1.294	-1.294	-1.294	-1.294	-1.292	-1.291	-1.290	-1.290	-1.290	-1.289
Huckel eigenvalues -	-1.288	-1.287	-1.287	-1.287	-1.286	-1.286	-1.285	-1.285	-1.285	-1.285
Huckel eigenvalues -	-1.285	-1.283	-1.283	-1.283	-1.282	-1.282	-1.282	-1.281	-1.281	-1.280
Huckel eigenvalues -	-1.280	-1.279	-1.279	-1.278	-1.278	-1.276	-1.276	-1.276	-1.276	-1.274
Huckel eigenvalues -	-1.266	-1.266	-1.265	-1.265	-1.264	-1.264	-1.264	-1.264	-1.263	-1.263
Huckel eigenvalues -	-1.263	-1.263	-1.262	-1.262	-1.262	-1.262	-1.261	-1.261	-1.253	-1.252
Huckel eigenvalues -	-1.252	-1.252	-1.251	-1.251	-1.251	-1.251	-1.251	-1.251	-1.251	-1.251
Huckel eigenvalues -	-1.251	-1.251	-1.250	-1.250	-1.250	-1.250	-1.250	-1.250	-1.250	-1.250
Huckel eigenvalues -	-1.250	-1.250	-1.250	-1.250	-1.250	-1.250	-1.250	-1.250	-1.250	-1.249
Huckel eigenvalues -	-1.249	-1.249	-1.249	-1.248	-1.244	-1.244	-1.206	-1.198	-1.198	-1.197
Huckel eigenvalues -	-1.192	-1.192	-1.192	-1.191	-1.191	-1.191	-1.151	-1.151	-1.150	-1.150
Huckel eigenvalues -	-1.150	-1.149	-1.149	-1.149	-1.149	-1.148	-1.148	-1.143	-1.143	-1.143
Huckel eigenvalues -	-1.136	-1.125	-1.125	-1.125	-1.104	-1.100	-1.100	-1.099	-1.097	-1.097
Huckel eigenvalues -	-1.097	-1.097	-1.096	-1.066	-1.065	-1.064	-1.064	-1.064	-1.064	-1.051
Huckel eigenvalues -	-1.047	-1.047	-1.047	-1.042	-1.038	-1.038	-1.038	-1.034	-1.023	-1.023

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## RESULTS AND DISCUSSION

We used different force field to determination of energy and other type of geometrical parameters, on the particular SWCNT, Because of the differences among force fields, the energy of a molecule calculated using two different force fields will not be the same (Fig.1).

In the process of investigating the combination of Thymine dimer coupling and CNT to achieve more information about these important gene systems, we attempted to construct different sequences of DNA (Thymine dimer section) include three nucleotides with these sequences: TTG, TGT, TTT and link them individually to outer surface of SWCNT to develop practical application of Thymine dimer coupling inside the SWNTs. These coupling have been performed between N atom of NH<sub>2</sub> groups of nucleotide T in TTT sequence of DNA, nucleotide T in TGT and TTG sequence of mRNA and nucleotide C in CAG sequence of mRNA with C atom in SWCNT. In Fig.2 and Fig3 and Fig4

the couplings between these sequences of DNA atoms with outer surface of SWNT have been displayed. Optimizations of these structures have been performed by using UFF and AM1 and DFT<sup>71</sup>.

So, it is not reasonable to compare the energy of one molecule calculated with a particular force field with the energy of another molecule calculated using a different force field. In this study difference in force field illustrated by comparing the energy of calculated by using force fields, MM+, Amber and OPLS. Theoretical energy values using different force fields, which is the combination of attraction van der Waals forces due to dipole-dipole interactions and empirical repulsive forces due to Pauli repulsion has been demonstrated in Table1 and Fig.2. Since the solute dipole moment induces a dipole moment in opposite direction in the surrounding medium.

Also, the energies have compared to the gas phase total energy CNT at the B1LYP/3-21G level of theory and different solvents and the graph

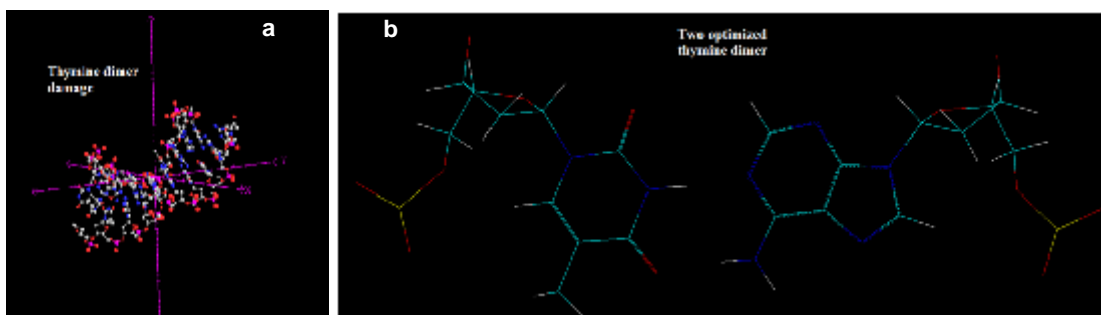


Fig. 1: (a) Thymine dimer damage (b) Two Thymine optimized

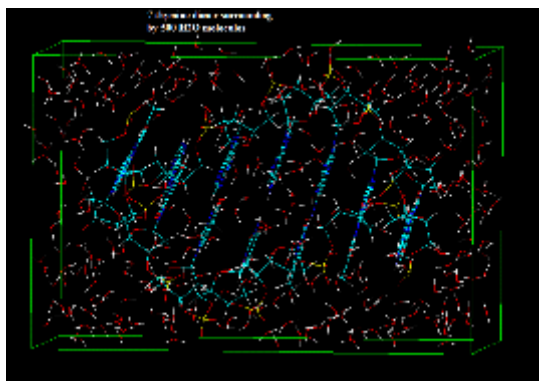


Fig.2. Thymine dimers surrounding with 500 H<sub>2</sub>O

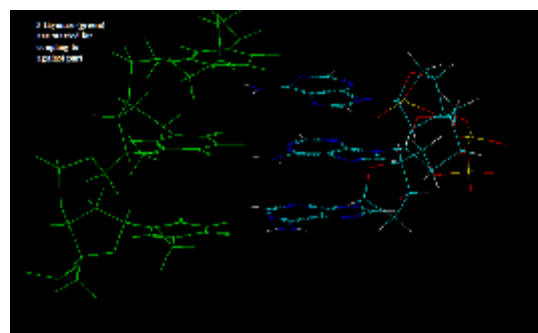


Fig. 3: Coupling of 3 thymine dimer

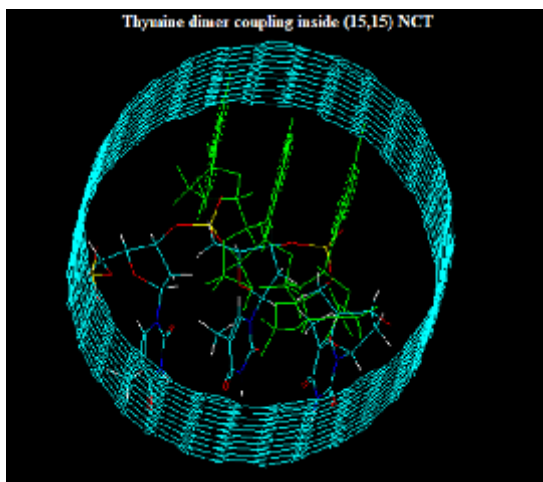


Fig. 4: Thymine dimer coupling inside the (15, 15) NCT

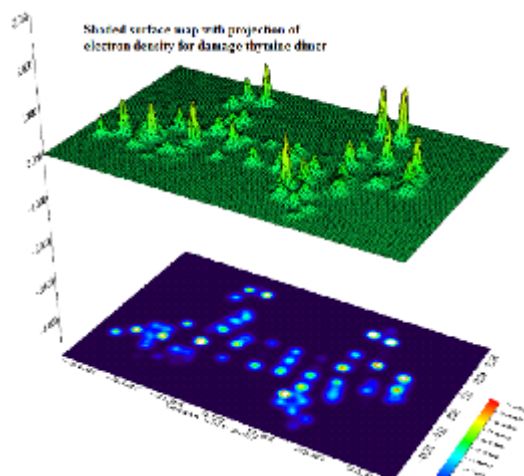


Fig. 5: Shaded Surface map with projection for electron density of thymine dimer damaged

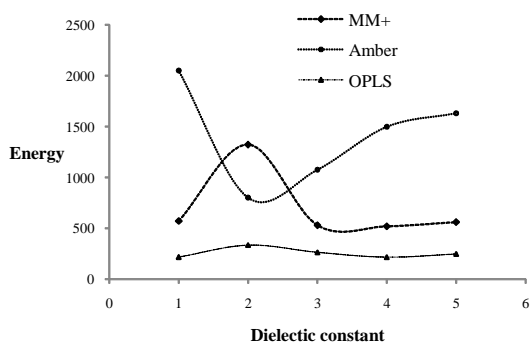


Fig. 6: The chart of optimized energy using theoretical methods in various media, which was reported in table 1.

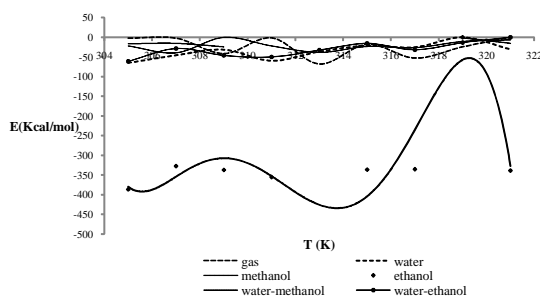


Fig. 7: Changes of relative energy versus temperatures in various media

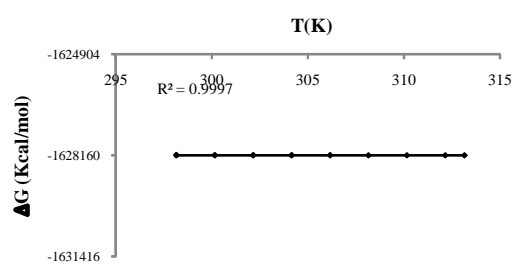
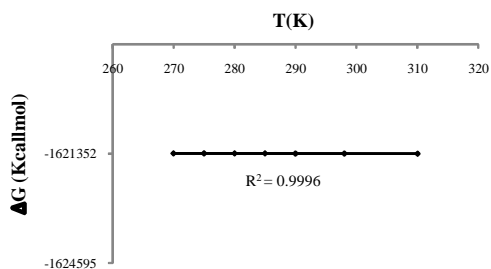


Fig. 5: (a) Thermodynamic Properties of SWCNT through the binding with Thymine dimer at different temperatures using STO-3G basis set in vacuum media, b) Gibbs free energies (Kcal/mol) in gas phase



of energy values versus dielectric constant of different solvents has been displayed at considered temperatures in Fig.3.

The GIAO (gauge independent atomic orbital) approximations of NMR calculations for Structural study of the combined systems of mRNA and CNT to obtain nuclei Magnetic Resonance

Parameters via Density Functional Theory (B3LYP) and Hartree Fock methods with STO-3G and 3-21G basis sets have been performed in gas phase too.

The results of NMR calculations consist of chemical shift anisotropy asymmetry ( $\eta$ ), isotropy ( $\sigma_{\text{iso}}$ ), anisotropy ( $\sigma_{\text{aniso}}$ ), and  $\Delta\delta$  and chemical shift tensor ( $\delta$ ) parameters have been obtained and reported in Tables 3.

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