

# The in Silico Insight into Carbon Nanotube and Nucleic Acid Bases Interaction

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## Abstract

**Background:** To explore practical applications of carbon nanotubes (CNTs) in biomedical fields the properties of their interaction with biomolecules must be revealed. Recent years, the interaction of CNTs with biomolecules is a subject of research interest for practical applications so that previous research explored that CNTs have complementary structure properties with single strand DNA (ssDNA).

**Objectives:** Hence, the quantum mechanics (QM) method based on ab initio was used for this purpose. Therefore values of binding energy, charge distribution, electronic energy and other physical properties of interaction were studied for interaction of nucleic acid bases and SCNT.

**Materials and Methods:** In this study, the interaction between nucleic acid bases and a (4, 4) single-walled carbon nanotube (SCNT) were investigated through calculations within quantum mechanics (QM) method at theoretical level of Hartree-Fock (HF) method using 6-31G basis set. Hence, the physical properties such as electronic energy, total dipole moment, charge distributions and binding energy of nucleic acid bases interaction with SCNT were investigated based on HF method.

**Results:** It has been found that the guanine base adsorption is bound stronger to the outer surface of nanotube in comparison to the other bases, consistent with the recent theoretical studies. In the other words, the results explored that guanine interaction with SCNT has optimum level of electronic energy so that their interaction is stable. Also, the calculations illustrated that SCNT interact to nucleic acid bases by noncovalent interaction because of charge distribution an electrostatic area is created in place of interaction.

**Conclusions:** Consequently, small diameter SCNT interaction with nucleic acid bases is noncovalent. Also, the results revealed that small diameter SCNT interaction especially SCNT (4, 4) with nucleic acid bases can be useful in practical application area of biomedical fields such detection and drug delivery.

**Keywords:** Carbon Nanotube, Nucleic Acid Base, Interaction, Binding Energy

## 1. Background

Recent years, the interaction of carbon nano tubes (CNTs) with biomolecules is a subject of research interest so that previous research explored that CNTs have complementary structure properties with Single Strand DNA (ssDNA) (1-3). The CNTs are divided to two kinds, single walled carbon nanotubes (SCNT) and multi walled carbon nanotubes (MCNTs). CNTs are classified in the three types based on the pair of integers of (n, m) that is related to the chiral vector. Hence, the types of CNTs are chiral ( $n = m$ ), arm-chair ( $n \neq m$ ) and zigzag ( $n, m = 0$ ) (4-9). Previous studies illustrated that SCNTs because of their molecular size, electronic structure and electrical conductivity are considered as a compatible candidate for binding to the polymers and biomolecules such as DNA (10-13). Although, previous lit-

eratures explored that SCNTs can bind to DNA by covalent and non-covalent conjugations but many details remain about this binding due to presence of various mechanisms on how they are connected (14-16). Many works have been done for demonstration details of SCNTs binding to DNA so that they reported the interaction between them mainly involve  $\pi$  orbitals of the C atoms in SCNT and base atoms (17, 18). However, there are still many questions about physical properties of SCNTs interaction with DNA. In this paper, we investigated nucleic acid bases interaction with SCNT (4, 4) for demonstration of physical properties of binding.

## 2. Objectives

Hence, the quantum mechanics (QM) method based on ab initio was used for this purpose. Therefore values

of binding energy, charge distribution, electronic energy and other physical properties of interaction were studied for interaction of nucleic acid bases and SCNT (4, 4).

### 3. Materials and Methods

#### 3.1. Computational Methods

In this work, for the investigating of SCNT interaction with nucleic acid bases (A, G, C, T) the complex of SCNT-base was modeled by Hyperchem 8.0.6 program (19) using OPLS force field that is given by following (Equation 1) (20):

$$E(r_{ij}) = E_{\text{bonds}} + E_{\text{angles}} + E_{\text{torsions}} + E_{\text{non-bonded}} \quad (1)$$

Also, for the molecular optimizations of SCNT, nucleic acid bases and complex of SCNT-base the QM calculations were performed. The Hartree-Fock method as an ab initio method that implemented in Gaussian 98 (17) was used for the molecular optimizations and QM studies. Furthermore, the physical properties of SCNT interaction with nucleic acid bases were calculated based on this method at theoretical level of 6-31G. Hence, the SCNT interaction with nucleic acid bases have been characterized by compare between electronic energy, atomic charge distribution and total dipole moment. The energy of binding was evaluated based on following (Equation 2) (21):

$$E_{\text{binding}} = E_{\text{SCNT-base}} - E_{\text{SCNT}} - E_{\text{base}} \quad (2)$$

Hence, in this work, the physical properties of interaction such as electronic energy, total dipole moment and binding energy of SCNT (4, 4) interaction with nucleic acid bases were determined using QM calculations based on Hartree-Fock method.

### 4. Results

Many works have been done to demonstrate details of SCNT interaction with ssDNA for various aims. In this work we investigated SCNT (4, 4) interaction with nucleic acid bases by theoretical method so that illustrated physical properties of interaction in order to practical functionality in biomedical field. The geometry optimization of SCNT-base complexes have been shown in (The results of calculations revealed that the complex between guanine and SCNT has optimum level of electronic energy rather than others. The values of electronic energy were summarized in (Table 1).

However, in order to stability evaluation of SCNT-base complex the binding energy of interaction was calculated based on Equation 2. The results of binding energy calculations explored that the complex of guanine and SCNT is

Table 1. Electronic Energy for Complex of SCNT-Base

Complex of SCNT-Base	E, kcal/mole
SCNT/adenine	$-21.88 \times 10^5$
SCNT/Guanine	$-22.35 \times 10^5$
SCNT/Cytosine	$-21.43 \times 10^5$
SCNT/Thymine	$-21.79 \times 10^5$

stable rather than others so that in view of the binding energy strength of bases to SCNT were ordered  $G > A > T > C$ . The values of binding energy were summarized in Table 2. These results are in fine agreement with previous study (21, 22).

Table 2. Binding Energy of SCNT-Base Complexes

Complex of SCNT-Base	Binding Energy, kcal/mol
SCNT/adenine	-75.81
SCNT/Guanine	-101.58
SCNT/Cytosine	-53.27
SCNT/Thymine	-71.35

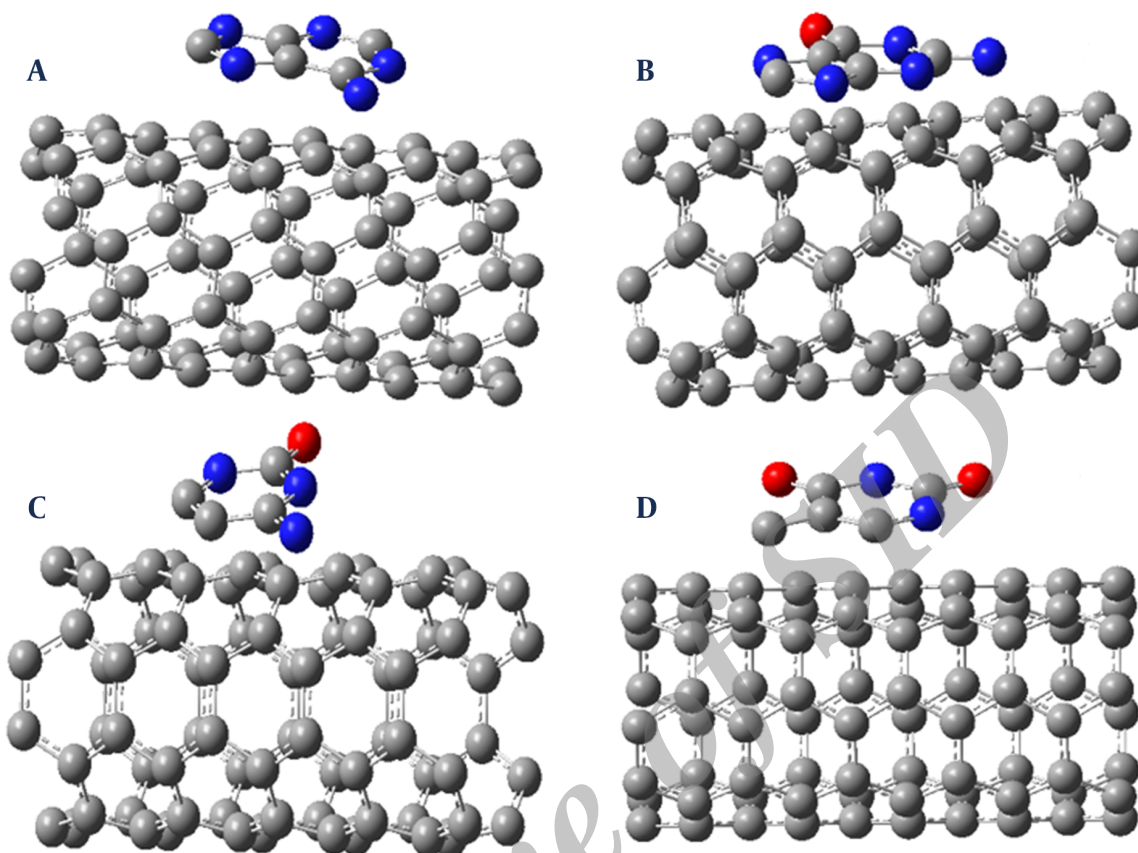
Also, the charge distribution calculations show that there is an electrostatic area in interaction situation of SCNT with nucleic acid bases. Hence, the results of charge distribution explored that interaction between SCNT and nucleic acid bases is noncovalent. The results of charge distribution calculation for guanine and SCNT complex is shown in (Figure 2). However, these results are confirmed by the values of total dipole moment of SCNT-base complexes. According to (Table 3) complex of SCNT and guanine has maximum value of total dipole moment so that for this complex in comparison with others a strength electrostatic area was created in place of interaction.

Table 3. Total Dipole Moment of SCNT-Base Complexes

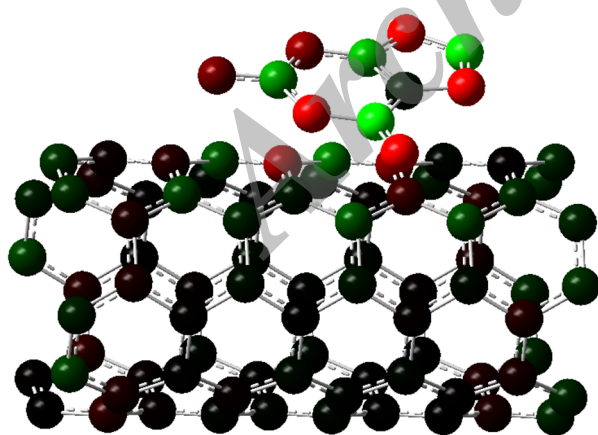
Complex of SCNT-Base	Total Dipole Moment, Debye
SCNT/adenine	13.93
SCNT/Guanine	14.96
SCNT/Cytosine	11.61
SCNT/Thymine	12.77

### 5. Discussion

Consequently, in this study we investigated SCNT (4, 4) interaction with nucleic acid bases. Our results re-



**Figure 1.** SCNT (4, 4) Interaction With (a) Adenine, (b) Guanine, (c) Cytosine and (d) Thymine



**Figure 2.** Plot of Charge Distribution in Place of Interaction for Guanine and SCNT Complex

vealed that complex of guanine-SCNT in comparison with

other complex is the most stable. Also the total dipole moment value and charge distribution exhibited a particular charge in place of interaction of guanine with SCNT. Furthermore, the results explored that the noncovalent interaction occur between SCNT and nucleic acid bases. Therefore, it can be concluded that small-diameter carbon nanotubes are suitable candidate for presence in treatment area especially drug delivery and detection of biomolecules in biomedical field.

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#### Footnotes

**Authors' Contribution:** Study concept and design, acquisition of data, analysis and interpretation of data: Dr. Behafarid Ghalandari; drafting of the manuscript, critical re-

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