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Computational Studies on the Interaction between Histidine and Single-Walled Carbon Nanotube; Concern to Electronic Structure

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Computational studies on the electronic structure of the Histidine (His) and Single-walled carbon nanotubes (SWCNT) were done using HF/6-31G method before and after interaction. These calculations showed that interactions are week. HOMO and LUMO and atomic charges studies proved that no charge transfer interaction was in the interactions. We have used the zigzag (7, 0) single wall carbon nanotube with a length of 20Å and zwitterions through the charged carboxylate and amine groups.

Keywords: Computational study, SWCNT, Histidine, Electronic Properties

1. INTRODUCTION

Single-walled carbon nanotubes (SWNTs) have potential biological and biochemical applications ranging from biomedical sensors to tissue supports to drug delivery [1-3]. Recently the interaction between amino acid and base paires with carbon nanotubes (SWCNTs) has been the focus of much attention due to their functionality in biological systems [4-5].

Due to the small size of the nanomaterials, they can penetrate and travel to different parts of body causing tissue injury. They may also deposit to undesirable and highly protected many parts of human system. In addition, they could pollute environment by increasing the concentration of nanoparticles in air, at least in the localized region. Nanoparticles (nanomaterials) can also cause allergic reactions to human and may enter into the food chain cycle. Nanomaterials or nanoparticles

including carbon nanotubes, upon prolonged exposure, can also cause asbestosis type of diseases in human [6-8]. So, interaction between amino acids and nanoparticles are very interesting.

One of the major areas of SWCNT research is the field of biomedical materials and devices special in drug delivery. Many applications for SWCNT have been proposed including biosensors, drug, and vaccine delivery vehicles and novel biomaterials [9].

However, the nature of biological-nanotube interactions is less well known, and this knowledge will be important in understanding their environmental and biological activity as well as their potential for application to nanostructure fabrication. Recently, adsorption of the glycine on (3, 3) armchair SWCNTs has been investigated through calculations based on density functional theory (DFT) [10]. Rajesh et al reported a study on the interaction between four amino acids with SWCNT [11]. In the recent years computational methods were applied in different branches of chemistry [12-26].

Prediction of the interaction strength between amino acids and nanotubes with changes in electronic structures is very important. In the present work, we have considered the electronic properties (atomic charges , HOMO and LUMO and dipole moment) before and after interaction between Histidine and the zigzag (7, 0) single wall carbon nanotube.

2. COMPUTATIONAL DETAILS

The structure of histinie and SWCNT were fully optimized by HF with the 6-31G basis set. A complex between Histidine and SWCNT were also fully optimized. To begin with, the gas phase geometry of Histidine was fully optimized. Full geometry optimizations and frequency calculations were performed and each species was found to be at minima, by having no negative values in the frequency calculation. Once the optimized geometries of the Histidine molecule and SWCNT are established adsorption of the aromatic rings on the substrate and SWCNT was carried out. Initially, for full geometry optimization, the aromatic ring of Histidine were placed in parallel to the SWCNT at a height of 4.0 Å, and allowed to relax freely.

The highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO) and dipole moment calculated at HF level in 6- 31G basis set, were summarized in Table 1. All calculation was performed using the Gaussian 98 program package [27].

3. RESULTS AND DISCUSSION

Optimized structures of the His, SWCNT and SWCNT–HIS complex is shown in Fig. 1, 2 and 3. It is evident that SWCNT–His complex is formed by the stacking interaction between the Histidine and the SWCNT.

The optimized distances between the aromatic ring plane of Histidine and the SWCNT were done. The lowest energy structure thus obtained was reoptimized to obtain the most favored configurations, which are shown in Fig. 3. Moreover, we note that the geometrical parameters such as

bond lengths and bond angles of the Histidine and SWCNT molecules remain almost unaltered even after the interaction with together. The C–C bond length was found to be 1.48 Å which is found to be consistent with previous observations [28-29].

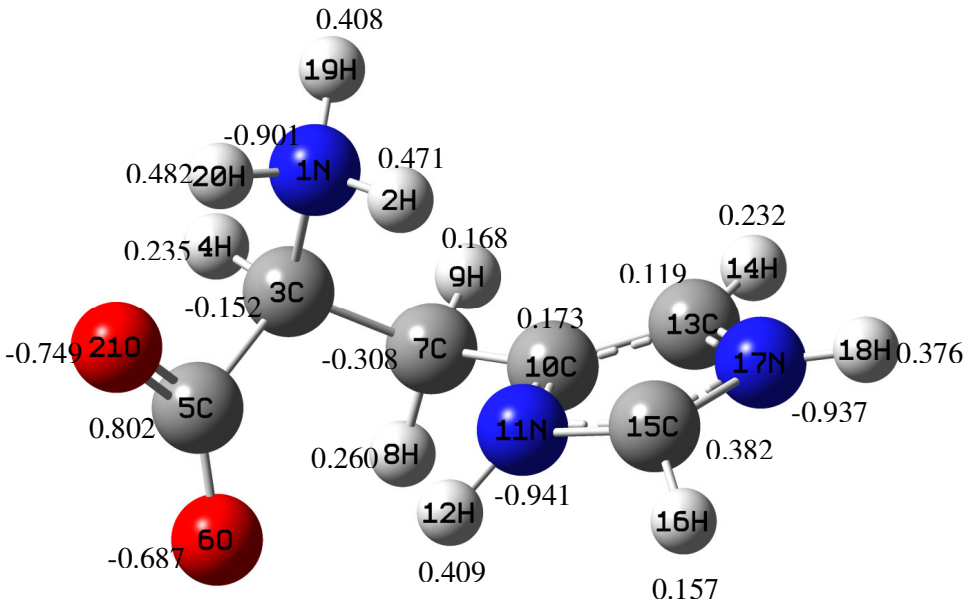

Figure 1. Optimized structure and atomic charges of Histidine before and after the complex formation (Parentheses include the changes after the complex formation)

This is attributed to the weak interaction between these systems. The goal is to investigate the changes in the HOMO, LUMO, dipole moment and atomic charges after interaction. Table 1 show the HOMO, LUMO and dipole moment of Histidine, SWCNT and SWCNT–His complex. Since, HOMO and LUMO energies of the Histidine and SWCNT are not close, charge transfer interaction did not occur. Although effect of Histidine on the HOMO and LUMO energies of the SWCNT is very low and is not significant.

Table 1. Dipole moment [D], HOMO and LUMO energies (in eV) of the Histidine, SWCNT and His-SWCNT complex

Compound	HOMO	LUMO	Dipole moment
His	-6.25	4.08	10.68
SWCNT	-4.62	-0.81	8.62
His-SWCNT	-4.62	-1.08	18.81

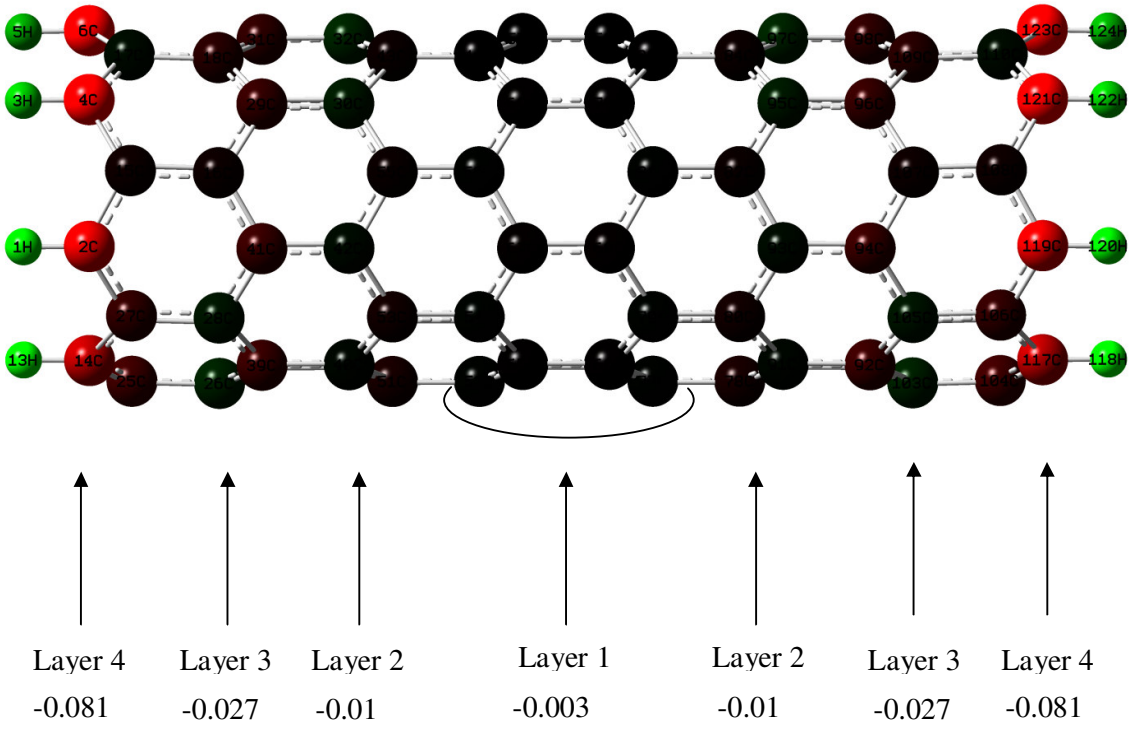

Figure 2. Optimized structure and average layer charges of SWCNT before the complex formation

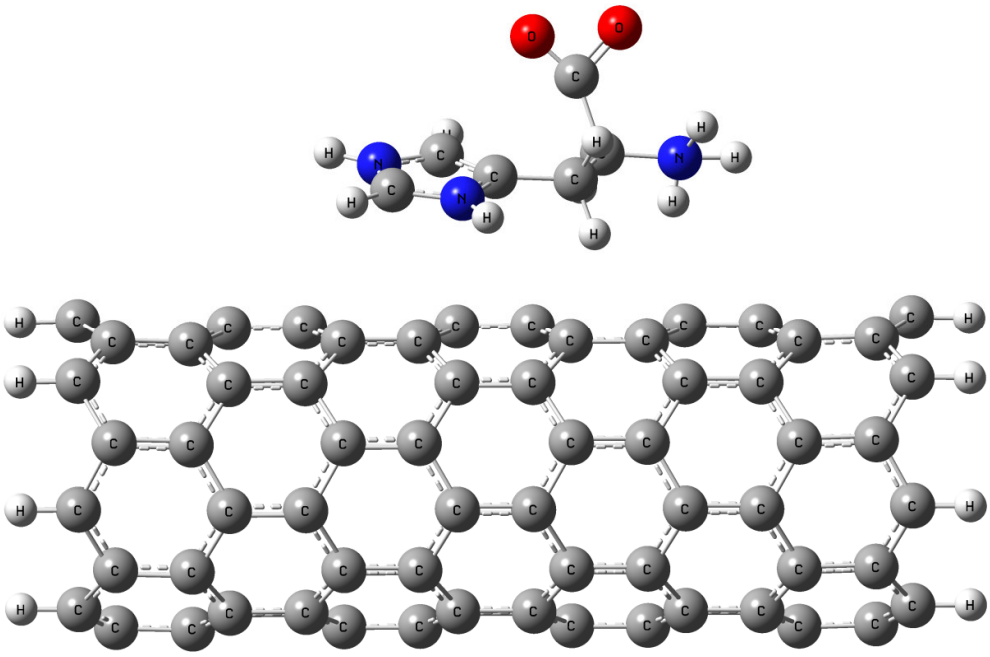

Figure 3. The full optimized structure of Histidine-SWCNT

The study of atom charges in SWCNT and SWCNT–His show that changes in atomic charges are law that shows interaction between SWCNT and His is week. Atomic charges for SWCNT and His are shown in Figures 1 and 2. Colors of the atoms in Figure 2 show the amount of charges. For example carbon atoms in layer 4 that have the most negative charges are red.

4. CONCLUSIONS

HF calculation with 6-31G basis set were performed for His-SWNT complex to obtained Mulliken charges, bond length, dipole moment and HOMO and LUMO energy. These results clearly indicated that electronic structures can be used for prediction of strength interactions between amino acids and SWCNT. In addition, there aren't charge transfer interactions between amino acids and SWCNT.

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References

1. A. Bianco, K. Kostarelos and M. Prato, *Curr. Opin. Chem. Biol.,* 9 (2005) 674
2. C. R. Martin and P. Kohli, *Nat. Re*V. *Drug Disco*V*ery,* 2 (2003) 29
3. J. Li, H. T. Ng and H. Chen, *Methods Mol. Biol.,* 300 (2005) 191
4. B. C. Baguley, *Anti-Cancer Drug Des.,* 6 (1991) 1
5. T. Roman, W. A. Di˜no, H. Nakanishi and H. Kasai, *Eur. Phys. J. D,* 38 (2006) 117
6. G. Oberdorster, E. Oberdorster and J. Oberdorster, *Environ. Health Perspect.,* 113 (2005) 823
7. N. Lewinski, V. Colvin and R. Drezek, *Small,* 4 (2008) 26
8. A. Takagi, A. Hirose, T. Nishimura, N. Fukumori, A. Ogata, N. Ohashi, S. Kitajima and J. Kanno, *J. Toxicol. Sci.,* 33 (2008) 105
9. S. K. Smart, A. I. Cassady, G. Q. Lu and D. J. Martin, *Carbon,* 44 (2006) 1034
10. T. Roman, W. A. Dino, H. Nakanishi and H. Kasai, *Thin Solid Films,* 509 (2006) 218
11. C. Rajesh, C. M. H. Mizuseki and Y. Kawazoe, *J. Chem. Phys.,* 130 (2009) 124911
12. S. Riahi, A. B. Moghaddam, M. R. Ganjali, P. Norouzi and M. Latifi, *J. Theor. Comput. Chem. (JTCC),* 6 (2007) 255
13. S. Riahi, P. Norouzi, A. B. Moghaddam, M. R. Ganjali, G. R. Karimipour and H. Sharghi, *Chem. Phys.* 337 (2007) 33
14. S. Riahi, A. B. Moghaddam, M. R. Ganjali and P. Norouzi, *J. Mol. Struct. (THEOCHEM),* 814 (2007) 131
15. S. Riahi, M. R. Ganjali, P. Norouzi and F. Jafari, *Sens. Actuators B,* 132 (2008) 13
16. S. Riahi, A. Beheshti, M. R. Ganjali and P. Norouzi, *Spectrochim. Acta Part A,* 74 (2009) 1077
17. M. R. Ganjali, A. Alipour, S. Riahi, B. Larijani and P. Norouzi, *Int. J. Electrochem. Sci.,* 4 (2009) 1262
18. Riahi, M. R. Ganjali, A. B. Moghaddam and P. Norouzi, *J. Theor. Comput. Chem. (JTCC),* 6 (2007) 331
19. S. Riahi, M. R. Ganjali, A. B. Moghaddam and P. Norouzi, *J. Theor. Comput Chem. (JTCC),* 6 (2007) 255
20. S. Riahi, S. Eynollahi and M. R. Ganjali, *Int. J. Electrochem. Sci.,* 4 (2009) 1407

21. S. Riahi, S. Eynollahi and M. R. Ganjali, *Int. J. Electrochem. Sci.,* 4 (2009) 1128
22. S. Riahi, S. Eynollahi and M. R. Ganjali, *Int. J. Electrochem. Sci.,* 4 (2009) 551
23. M. R. Ganjali, T. Razavi, F. Faridbod, S. Riahi and P. Norouzi, *Curr. Pharm. Anal.*, 5 (2009) 28
24. S. Riahi, P. Pourhossein, A. Zolfaghari, M. R. Ganjali and H. Z. Jooya, *Fuller Nanotub Car. N,* 17 (2009) 159
25. F. Faridbod, M. R. Ganjali, R. Dinarvand, S. Riahi and P. Norouzi, *J. Food Drug Anal.*, 17 (2009) 264
26. S. Riahi, S. Eynollahi, M. R. Ganjali and P. Norouzi, *Int. J. Electrochem. Sci.,* 5 (2010) 355
27. M. J. Frisch, G. W. Trucks, H. B. Schlegel and et al., Gaussian Inc. Pittsburgh, PA (1998)
28. R. Saito, G. Dresselhaus and M. S. Dresselhaus, *Physical Properties of Carbon Nanotubes,* Imperial College Press, London (1998)
29. M. S. Dresselhaus, G. Dresselhaus and P. C. Eklund, *Science of Fullerenes and Carbon Nanotubes,* Academic, San Diego (1996)