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Full Length Research Paper

Transportation of single wall carbon nanotube (SWCNT) through the cell membrane

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Carbon nanotubes (CNTs) are very common in medical research and are being highly studied in the fields of biosensing methods for disease treatment and efficient drug delivery and health monitoring. The transportation of open-end Single wall carbon nanotube (SWCNT) through the cell membrane widely investigated because of many advantages. In our recent study, extensive quantum mechanical (QM) calculation of electronic structure of open-end of SWCNT and transportation of single wall carbon nanotube through the cell membrane have been administered in vacuum media using GAUSSIAN 98 software. Our results manifested that the interaction of open-end of SWCNT has minimum value of energy interaction and then most structural stability in vacuum. We assayed effects of vacuum on transportation of SWCNT through the cell membrane with using B1LYP and Hartree Fock (HF) methods at STO-3G, 3-21G, 6-31G levels of theory. Also, we demonstrated the total atomic charges of dense region calculated STO-3G, 3-21G and 6-31G basis sets in vacuum with HF method. The calculated values showed negative charge at this site. The O and S atoms at interaction site produced negative charge because they have high electron affinity.

Key words: Single wall carbon nanotube (SWCNT), quantum mechanical (QM), STO-3G, 3-21G and 6-31G basis.

INTRODUCTION

Kroto et al. (1985) first reported the existence of buckminsterfullerene C60, theoretical speculation about carbon clusters (Dornenburg and Hintenberger, 1989) over 36 years was finally verified. Since then, this beautiful molecule has attracted ever more attention of theoretical and experimental scientists. Some chemists began to focus their research on the chemistry of this molecule, but real fullerene chemistry began only after 1990 when Kratschmer et al. described a method for preparing macroscopic quantities of C60 (Kratschmer et al., 1990). Then many polymer scientists shifted their attention to this field. They tried to use this molecule as a building block to construct novel materials with unusual properties. The discovery of carbon nanotubes (CNT) in 1991 heralded the era of nanoscience and nanotechnology (Iijima, 1991). Nanotubes of carbon and other materials, due to their electronic, optical and mechanical properties find applications in several fields (Monajjemi et al., 2008, 2009, 2010, 2011). The space available inside the nanotube enables it to match phospholipids outside. This makes the carbon nanotube an ideal medium for storing high energy materials (Abou-Rachid et al., 2008), their discovery (Iijima, 1991) have been the focus of scientific research due to their outstanding chemical, mechanical and electrical properties. Single walled carbon nanotubes (SWCNTs) are of particular interest because of their size and superior electrical properties (Odom et al., 1998). They have been used to realize many molecular scale electronic devices (Monajjemi et al., 2010; Postma et al., 2001).

The recent observation that carbon nanotube enhances reaction rates inside the cage is promising (Pan et al., 2007). Since carbon nanotubes can exert substantial pressure inside, they may be considered as possible

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reaction vessels for such reactions (Pupysheva et al., 2008). Based on the reports of intake of molecules inside carbon nanotube (Cui et al., 2004; Eswaramoorthy et al., 1999; Hummer et al., 2001) they have also been proposed as means for ions delivery to the cells (Liu et al., 2008; Ghalandari et al., 2011; Hilder and Hill, 2008). CNT can be functionalized with bioactive peptides, proteins, nucleic acids and drugs, and used to deliver their cargos to cells and organs. Because functionalized CNT display low toxicity and are not immunogenic, such systems hold great potential in the field of nano-biotechnology and nanomedicine. There are two methods to deliver ions into the cells, both equally effective, (a) the ion can be attached to the side or behind, (b) or the ion can actually be placed inside the nanotube. Direct electron transfer between the electrode and the redox enzyme is very important for fundamental studies and construction of biosensors (Liang et al., 2010; Mollaamin et al., 2010; Albareda-Sirvent and Hart, 2002). However, the direct electron transfer between the enzyme and unmodified electrode is usually prohibited due to shielding of the redox active sites by the protein shells (Wang et al., 2008; Mollaamin et al., 2010). Therefore, several studies have been made to enhance the electron transfer. Mediators are widely used to access the redox center of an enzyme and then to act as the charge carriers. Mediators can minimize the effects of inter-ferences, lower the operating potential of the electrodes, and improve the linear response range and sensitivity of the sensor (Zhang et al., 2007). Use of carbon nanotubes (CNTs) as mediators has attracted increasing attention in recent years. Comparing with traditional carbon electrodes, CNTs show unique properties, such as good conductivity, high chemical stability, and catalytic activities towards many electrochemical reactions (Mollaamin et al., 2010; Wang et al., 2008; Manso et al., 2007; Jurkschat et al., 2006). More importantly, it is possible to bring the nanotubes close to the redox centers of the proteins (Gooding et al., 2003; Liu et al., 2005).

THEORETICAL METHODS

The calculations have been carried out by using the GAUSSIAN 98 suite of programs. The density functional theoretical method with the HF functional and the STO-3G, 3-21G, 6-31G basis set was used for all the calculations.

Hartree Fock (HF) implemented in calculations using STO-3G, 3-21G and 6-31G basis sets Gaussian 98 (Monajjemi et al., 2008) for the vacuum which provided logical precision and is particularly suitable for the study of deficiencies in a wide range of materials. There are several different HF functional, available differing elementarily in the choice of the basis functions, in which, the electronic wave functions are expanded and the scheme of integration.

Nuclear magnetic resonance (NMR) is based on the quantum mechanical property of nuclei. The chemical shielding refers to the phenomenon which attached with the secondary magnetic field created by the induced motions of the electrons that circling the nuclei when in the presence of an applied magnetic field for chemical shielding (CS) tensors, which describes how the size of shielding varies with molecular tendency, we often use the following convention for the three principle component:

$$\sigma 11 \leq \sigma 22 \leq \sigma 33$$

The three values of the shielding tensor are frequently represented as the isotropic value (σ_{iso}), the anisotropy shielding ($\Delta\sigma$), and the asymmetry parameter (η) (Monajjemi et al., 2008). In our current study, extensive quantum mechanical calculation of electronic structure of the cell membrane's phospholipids interaction with open-end of SWCNT and solvent effects on ^{13}C, ^{15}N, ^{17}O , ^{18}S , ^{1}H NMR parameters have been performed in vacuum media using GAUSSIAN 98 program.

RESULTS AND DISCUSSION

There are several experimental and theoretical results available on the structural of CNT, cell membrane and transferring CNT through the cell membrane. In the present study we carried out the CNT by the cell membrane which can form suitable supports for curing some disease. This section describes the characteristics of the SWCNT. In a previous work, we calculated the minimal basis sets of STO-3G, 3-21G, 6-31G in vacuum and solvents. In different ways, those atoms that had more distance from the nanotube's head connection and they were active atoms such as N1 , N25 , O46 , S47 , S55 have more over lab in the STO-3G, 3-21G, 6-31G basis set as the isotropic value (σ_{iso}) (Table 1 and Figure 1a) and the anisotropy shielding (Table 1 and Figure 1b). As it can be seen in Table 1 and Figure 1c, an important piece of information about $\Delta\sigma$. According to Table 1, and Figure 1d, N10, O8, S55 atoms have shown the highest shift when we calculated it for δ parameter. These atoms have active head and highest interaction with nanotube.

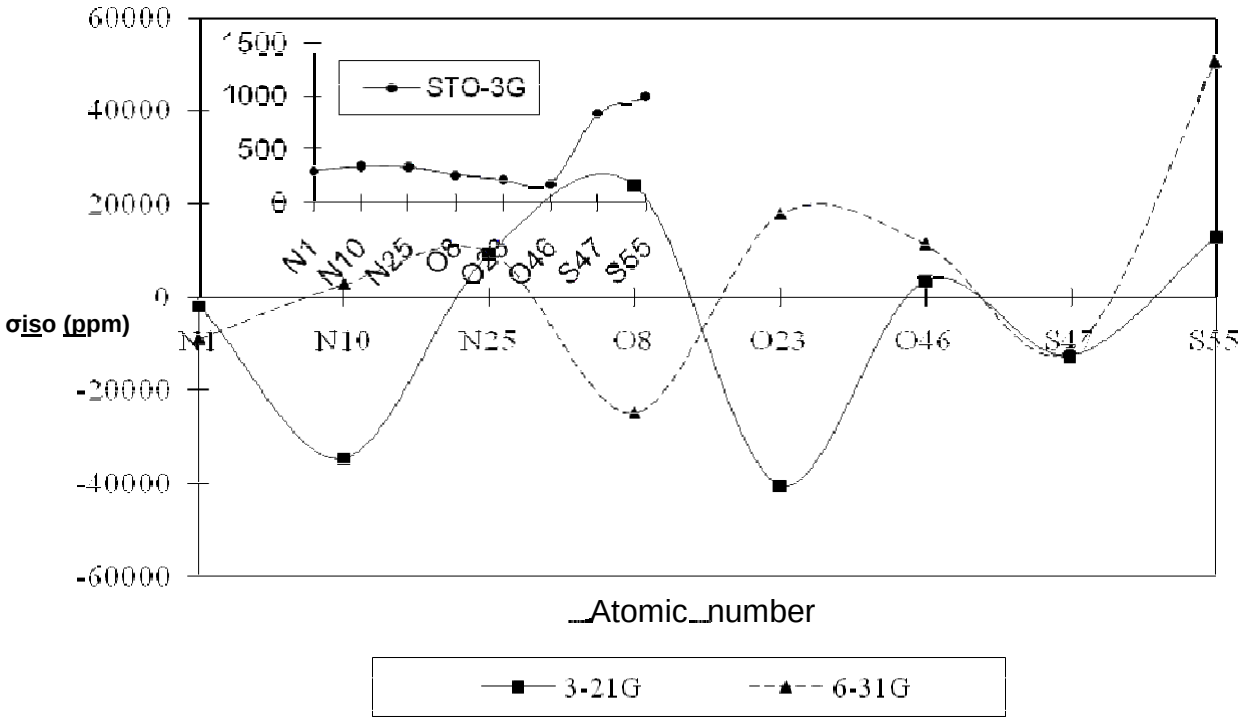
In Figure 2 we have shown the atomic charge's diagram calculated by B3LYP method using 6-31G, 3-21G and STO-3G basis sets in vacuum media (Table 2). The interaction between membrane's phospholipids has been displayed with open-end of SWCNT atoms. To describe this application of this interaction, the calculated physical properties have been investigated in vacuum which is important in molecular properties. In Figure 3a the interaction energy has vacuum optimum level. In this figure you can see how the temperature goes up and how the interaction energy is lift up. Also we can see this result in the interaction entropy (Figure 3b, but in the Gibbs free energy the result is completely different. In Figure 3c the Gibbs free energy decreases whilst the temperature increases.

Therefore, we have inferred the Correlation between ransportation of SWCNT through the cell membrane and the Gibbs free energy, entropy, enthalpy. According to the results**,** we can receive this formula:

G= H–T S G=0.06-0.134T

Table 1. The NMR parameters of S, N,O, H nuclei exist in the cell membrane's phospholipids interacted with open-end of SWCNT in vacuum media using STO-3G, 3-21G and 6-31G basis sets.

Atomic number	σiso				σaniso			Δσ			δ	
	3-21G	sto-3G	6-31G	3-21G	sto-3G	6-31G	3-21G	sto-3G	6-31G	3-21G	sto-3G	6-31G
N1	-1856.6	298.936	-9064.8	12788.64	61.7596	41782.97	8525.762	41.1731	27855.31	8525.762	41.1731	27855.37
N10	-34739	341.292	2795.95	67984.29	154.8934	58229.35	45322.86	103.2623	38819.57	45322.86	103.2623	38819.57
N25	9314.14	335.639	9835.53	9225.841	193.4408	14419.11	6150.56	128.9605	9612.741	6150.561	128.9605	9612.741
O8	24015.4	259.243	-24893	35906.24	140.1166	82253.69	23937.5	93.381	54835.79	35906.24	93.411	54835.79
O23	-40431	213.021	17840.2	74818.9	133.8407	20574.29	49879.27	10.0782	13716.19	49879.27	89.2271	13716.19
O46	3582.68	179.428	11367.4	283747.6	379.435	14249.87	89165.08	252.9567	9499.917	89165.08	252.9567	9499.917
S47	-12735	831.141	-11534	38227.6	276.6522	32884.33	25485.07	184.4348	21922.89	25485.07	184.4348	21922.88
S55	12935.2	986.654	50631.4	670714.6	663.1762	450679.8	46879.27	442.1175	300453.2	12925.84	442.1175	453.218



(a)

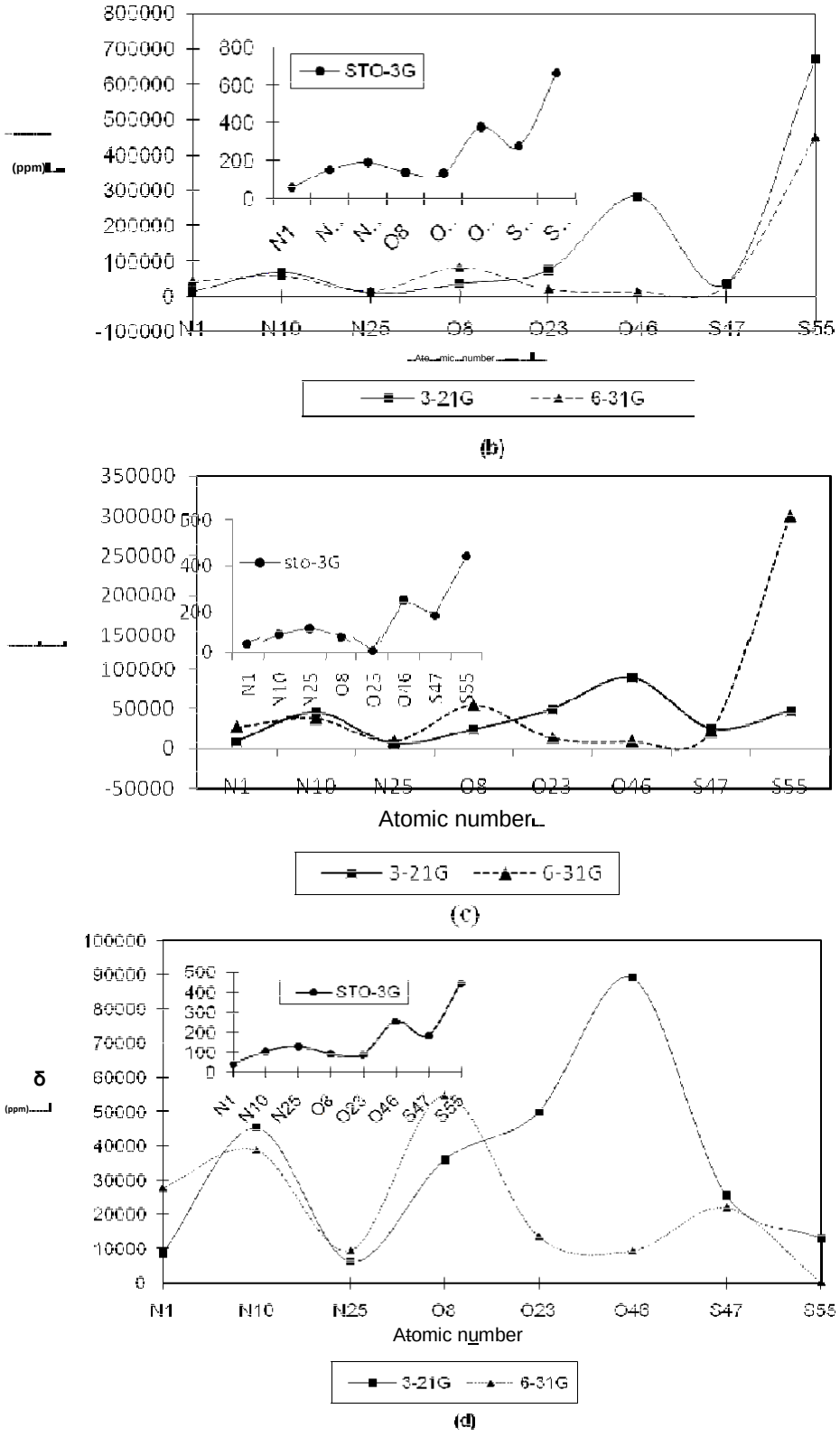


Figure 1. (a). The isotropic value calculated by B3LYP method using 6-31G, 3-21G and STO-3G basis sets in vacuum media, (b) The anisotropy shielding calculated by B3LYP method using 6-31G, 3-21G and STO-3G basis sets in vacuum media, (c) The Δσ shielding calculated by B3LYP method using 6-31G, 3-21G and STO-3G basis sets in vacuum media, (d) The δ parameter calculated by B3LYP method using 6-31G, 3-21G and STO-3G basis sets in vacuum media.

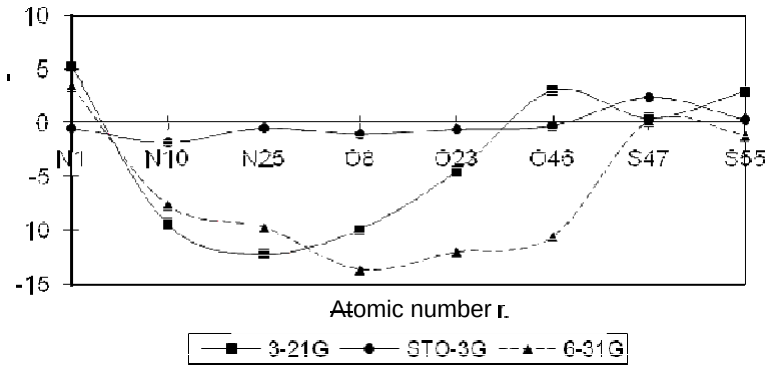


Figure 2. The atomic charges diagram calculated by B3LYP method using 6-31G, 3-21G and STO-3G basis sets in vacuum media.

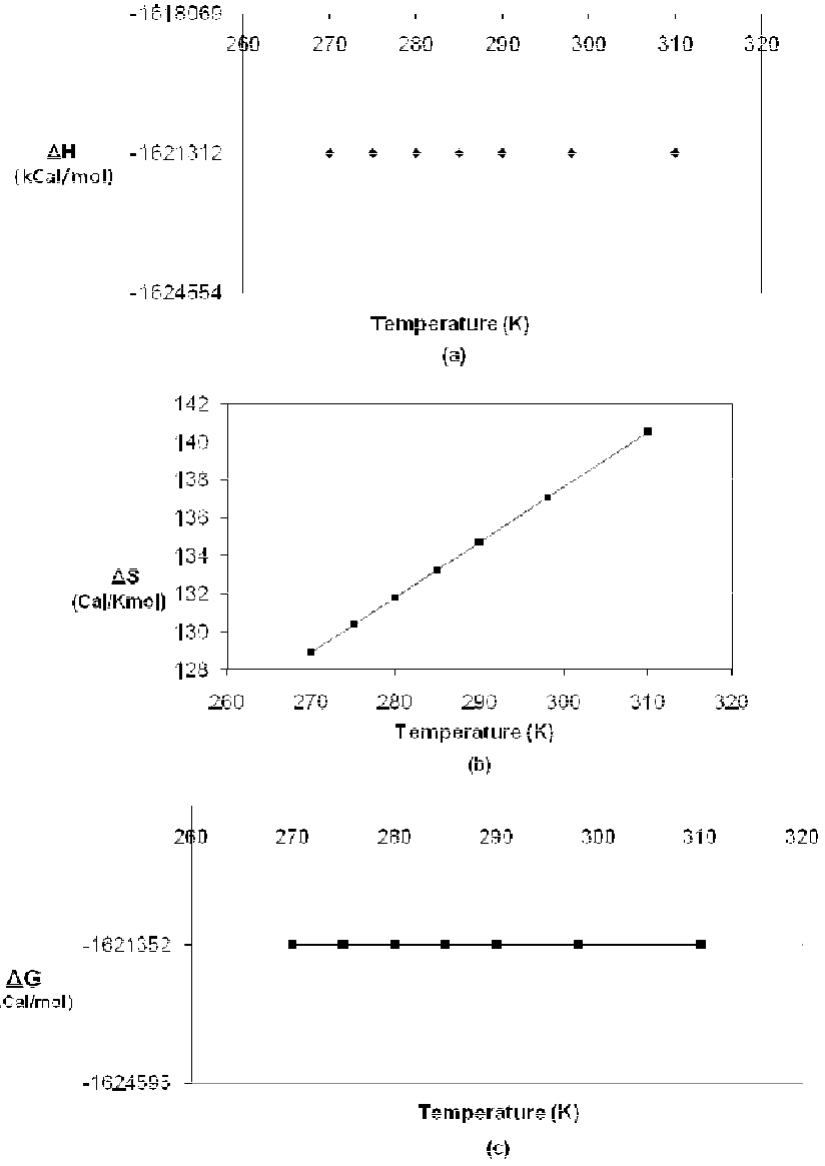


Figure 3. Thermodynamic properties of SW CNT through the cell membrane at different temperatures using STO-3G basis set in vacuum media.

Table 2. Total atomic charges (a.u.) calculated with B3LYP method using 6-31G, 3-21G and STO-3G basis sets in vacuum media.

Atomic number	Atomic charge		
	3-21G	sto-3G	6-31G
N1	5.195449	-0.50511	3.422102
N10	-9.43628	-1.80179	-7.65491
N25	-12.2285	-0.50606	-9.74001
O8	-9.92948	-1.10277	-13.6731
O23	-4.53749	-0.61129	-12.0375
O46	2.965146	-0.28655	-10.5983
S47	0.404502	2.335049	0.186649
S55	2.888076	0.266858	-1.16666

Table 3. The IR logistic in different temperature using STO-3G basis set in vacuum media.

Temperature (K)	H (kCal/mol)	S (Cal/Kmol)	G (kCal/mol)
270	-1621312	128.898	-1621347
275	-1621311	130.339	-1621347
280	-1621311	131.782	-1621348
285	-1621311	133.229	-1621349
290	-1621310	134.678	-1621349
298	-1621309	137.045	-1621350
310	-1621308	140.498	-1621352

$R^2 = 0.999$

Accordingly, it can be seen whilst the temperature increases, the Gibbs free energy decreases so we have a constant system. On the other hand with this kind of interaction, we could catch a good result for R^2 because it is near to number 1 (Table 3).

Conclusion

Recently carbon nanotubes have attracted increasing attention. The CNTs show unique properties, such as conductivity, chemical stability, and catalytic activities. In conclusion, we have showed the interaction between cell membrane's phospholipids and SWCNT to demonstrate the stability of cell membrane's phospholipids /SWCNT system. As expected, the NMR resolution shows the important impress of N1, N10, N25, O8, O46, S47 and S55 which is for our cell membrane, in the whole of our system.

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