

Studying physicochemical characteristics of Flutamide adsorption on the Zn doped SWCNT (5,5), using DFT and MO calculations

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Abstract

In this study, the adsorption of Flutamide (FLT) anticancer drug on the Zn doped single-walled carbon nanotube (5, 5) (SWCNT-Zn (5, 5)) has been investigated. This study has been examined in the gaseous phase and also in water and ethanol solvents phases, in the basis and excited states, using density functional theory (DFT) and molecular orbitals (MO) calculation methods. DFT calculations were performed at B3LYP quantum chemical level and at 6-311G (d, p) basis orbital set. In the first step, the structure of FLT was optimized at B3LYP/6-311G (d,p) theoretical level. The obtained results clearly demonstrate the energy stability of the optimized geometries and obviously show that the nature of Flutamide adsorption energy on the surface of SWCNT is in the range of the physisorption. Afterwards, the various structures of SWCNT (5, 5) and the adsorption of FLT on the outer surface of SWCNT (5, 5) was investigated using DFT method. The energies of FLT, SWCNT (5, 5), Zn doped SWCNT (5, 5), the energies of HOMO and LUMO orbitals, gap energy and dipole moments have been calculated using DFT and MO methods.

Keywords: Flutamide (FLT); SWCNT; DFT method; MO method; physisorption.

Introduction

Flutamide (FLT) (trade mark Eulexin) (4-nitro-3-fluoromethylisobutyramilide) is considered as the earliest attainable non-steroid antiandrogen recognized by the world as the most useful compound to treat prostate cancer. Several studies conducted in this case have been led to the reasonable and interesting results [1-4].

Single-walled carbon nanotubes (SWCNTs) and their prominent features in terms of chemical, electrical and 1 D structural properties pioneered in various major fields in science. Proved amazing and unique properties of these structure led to a widespread use of them in various categories of science, including medicine, industry and technology. Due to their inherent features, SWCNTs are able to not only

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deliver the bioactive molecules across cell membranes, but also into the cell nuclei because of their very high surface areas [5-8]. Certain theoretical studies on the behaviors of 1, 3-dipolar cycloadditions on the (n,n) SWCNTs have been performed and the results of this investigation have been reported by the authors [9]. The adsorption of several gaseous molecules on the surface of SWCNTs has been investigated using DFT method at B3LYP theoretical level and also the results of NMR data have been indicated [10, 11, and 12]. Some quantum chemistry theoretical investigations on the features of HOMO and LUMO orbitals and their energy gap in the polycyclic aromatic hydrocarbons and metal clusters have been provided the significant results [13,14]. Some physical chemistry characteristics of room temperature ionic liquids have been also studied and the results of its temperature dependence seems to be interesting [15]. In addition, NMR, NQR and the structural studies on nanotubes have been performed using DFT computational method [16-18].

Recently, several physicochemical properties of anticancer drugs adsorption characteristics and also drug delivery features have been studied using DFT and MD theoretical methods [19–21].

In this research, the adsorption of FLT (prostate specific antigen (PSA)) on the surface of carbon nanotubes (5, 5) has been investigated using density functional theory (DFT) and molecular orbitals (MO) methods. All calculations have been performed at B3LYP quantum chemical level and at 6-311G (d, p) basis set. Also, the interaction of FLT with Zn doped SWCNTs (5, 5) has been investigated.

After preparing the models and input files, the structures were optimized properly and the obtained results have been studied. Finally, to realize the drug effectively, the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), were obtained and studied. All the obtained results of these calculations are presented in the following tables and figures. The optimized structure of FLT is shown in Figure 1.

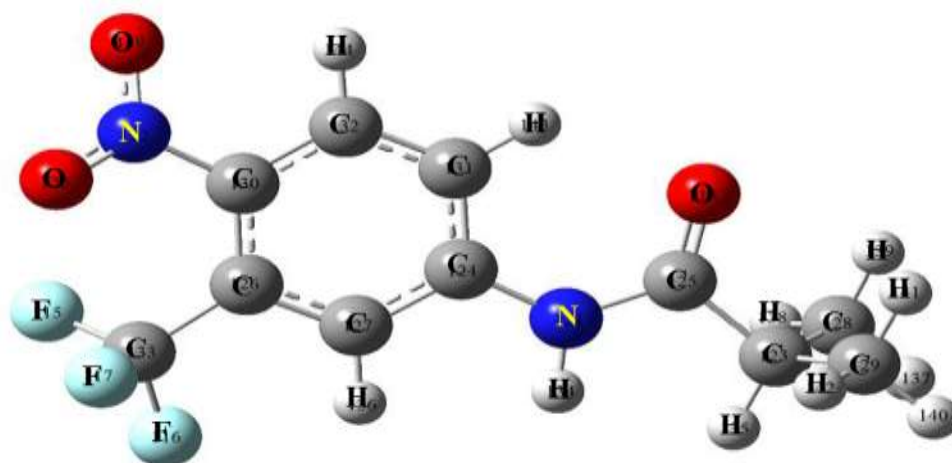


Figure 1. The optimized structure of FLT

Computational method

In this study, FLT anticancer drug and the interaction between SWNTs (5, 5)-Zn and FLT in the basis and excited states in the gaseous phase, also in the water and ethanol solvents, was investigated. Gaussian 09 program have been used for all computations [22]. All the figures were drawn using Gaussview software, and the calculations were performed using DFT method at B3LYP quantum chemical and at 6-311G (d, p) basis orbital set. Furthermore, molecular orbitals (MO) and magnetic resonance of the nucleus (NMR) calculations have been performed to get more data concerning energy gaps and dipole moments. The assumed carbon nanotube (5, 5) which was used in this study contains 90 carbon atoms where the open ends are saturated by hydrogen atoms. In this investigation, SWCNT (5,5) is considered as the target nanotubes because of its high reactivity, small diameter and also high pyramidalization angle which is an important parameter in the reactivity of nanotubes [6, 9, and 10].

Results and discussion

The comparison of energy and bipolarity of the drug in the both basis and excited states

The energies and dipole moments were computed in basis state (in the both gaseous and solvent phases) and the excited state (in gaseous phase) using

DFT method at B3LYP level and at 6-311G (d, p) basis set reported in Table 1. According to Table 1, in the gaseous phase, the energy in the excited state (-28856.576 eV) does not differ significantly the energy of basis state (-28856.007 eV). However, the drug is, more or less, more stable in the gaseous phase and excited state. The dipole moments in the gaseous phase and in the excited state is 4.33540 Debye(D) that is greater than the dipole moment in the same phase and in the basis state (3.4783 D). This fact may be attributed to the different distribution of electronic charges in the two mentioned states.

The energy of basis state in ethanol phase is -28864.07 eV, slightly greater than in the both gaseous and water solvent phases. This suggests that the drug may be more stable in the ethanol solvent phase than others. Moreover, the dipole moment in the basis states and in ethanol solvent phase is 4.7224 D, which is greater than in the water solvent phase (4.61604 D), in the gaseous phase (3.4783 D) and also in the excited state (4.3540 D). This phenomenon can also be attributed to the distribution of electronic charges in the orbitals. According to above results, the polarity of molecule affect its stability. Therefore, the stability of the molecule will be increased significantly by increasing the polarity of molecular structure.

Table 1. Energy and dipole moment of FLT calculated at B3LYP/6-311G (d, p) theoretical level

Phase	Basis state		Excited state	
	Dipole moment (D)	Energy (eV)	Dipole moment (D)	Energy (eV)
Gaseous	3.4783	-28856.007	4.3540	-28856.576
Water	4.6160	-28856.957	-	-
Ethanol	4.7224	-28864.075	-	-

Analysis of molecular orbitals (MO) at B3LYP theoretical level

In general, studying HOMO and LUMO energies is used to distinguish the charge transfer in the molecule. HOMO and LUMO orbitals are considered as essential parameters that clearly illustrate the ability of electron donating or electron accepting, respectively. Furthermore, the molecules with high HOMO energy are capable to lose easily their electrons, therefore, they can be considered as more reactive. As the same way, LUMO orbitals with a low energy level relative to the energy level of HOMO orbitals are capable to accept easily the electrons which have been transferred from HOMO orbitals. The energy difference between HOMO and LUMO orbitals (ΔE_{H-L}) is called the energy gap (E_g) that can be calculated by Equation 1.

$$E_g = \Delta E = E_{HOMO} - E_{LUMO} \quad (1)$$

The energy distance between these orbitals helps us to understand and clarify the kinetic stability and molecular reactivity of molecules, and furthermore, it is possible to study the intermolecular charge transfer. Knowing the energy gap also, can evaluate not only the chemical adsorption but also the electronic characteristics of species, effectively. In fact, the smaller energy distance indicates the more stable LUMO state, which is due to the higher capability of electron acceptance by this orbital. If the energy distance between HOMO and LUMO orbitals is small, therefore, the molecule will be very reactive, and consequently the higher charge transfer will occur and the reactivity increases. The results obtained from calculations at B3LYP/6-311G (d, p) theoretical level are shown in Table 2. This electron acceptance can be due to the electron transfer from HOMO orbital to the LUMO orbital in the basis state and is mainly described by an electron excitation from the HOMO orbital to the LUMO orbital.

Table 2. HOMO energy, LUMO energy and E_g (eV) at B3LYP/6-311G (d, p) theoretical level

Phase	Basis state			Excited state		
	E_{HOMO} (eV)	E_{LUMO} (eV)	E_g (eV)	E_{HOMO} (eV)	E_{LUMO} (eV)	E_g (eV)
Gaseous	-0.28867	-0.17516	0.11351	-0.27818	-0.09994	0.17824
Water	-0.28595	-0.18202	0.10393	-	-	-
Ethanol	-0.25837	-0.10350	0.15487	-	-	-

As can be seen in Table 2 and Figure 2 (DOS plots), both E_{HOMO} and E_{LUMO} in the excited state and in gaseous phase are higher than in the basis state. Also, the energy gap in the excited state is greater than the basis state. This may be interpreted by higher reactivity of FLT in basis state. The DOS plots are shown in Figure 2. The shape of the

HOMO and LUMO orbitals is also shown in Figures 3 and 4.

E_g in the excited state and in gaseous phase (0.17824 eV) is greater than the E_g in the basis state (0.11351 eV) and, as a consequence, the molecule is more stable in excited state and has the lower reactivity comparing to the basis state in gaseous phase. As seen in Figure 2,

and based on the obtained data, E_{HOMO} and E_{LUMO} in basis state in both gaseous and water solvent phases is more negative than in ethanol solvent phase. Whereas, E_g in ethanol solvent phase is greater than its value in both gaseous and water solvent phases. These results will lead to the consequence that the drug is more stable in ethanol phase and also less reactive. It seems that, the molecule in the water phase and in the

basis state with $E_g=0.10393$ eV has the lowest stability, the highest charge transfers and consequently the most reactivity.

A view of data analysis to obtain E_g , HOMO and LUMO

Diagrams 1 and 2 are a part of the Notepad output data and demonstrate that the E_{HOMO} and E_{LUMO} are attainable.

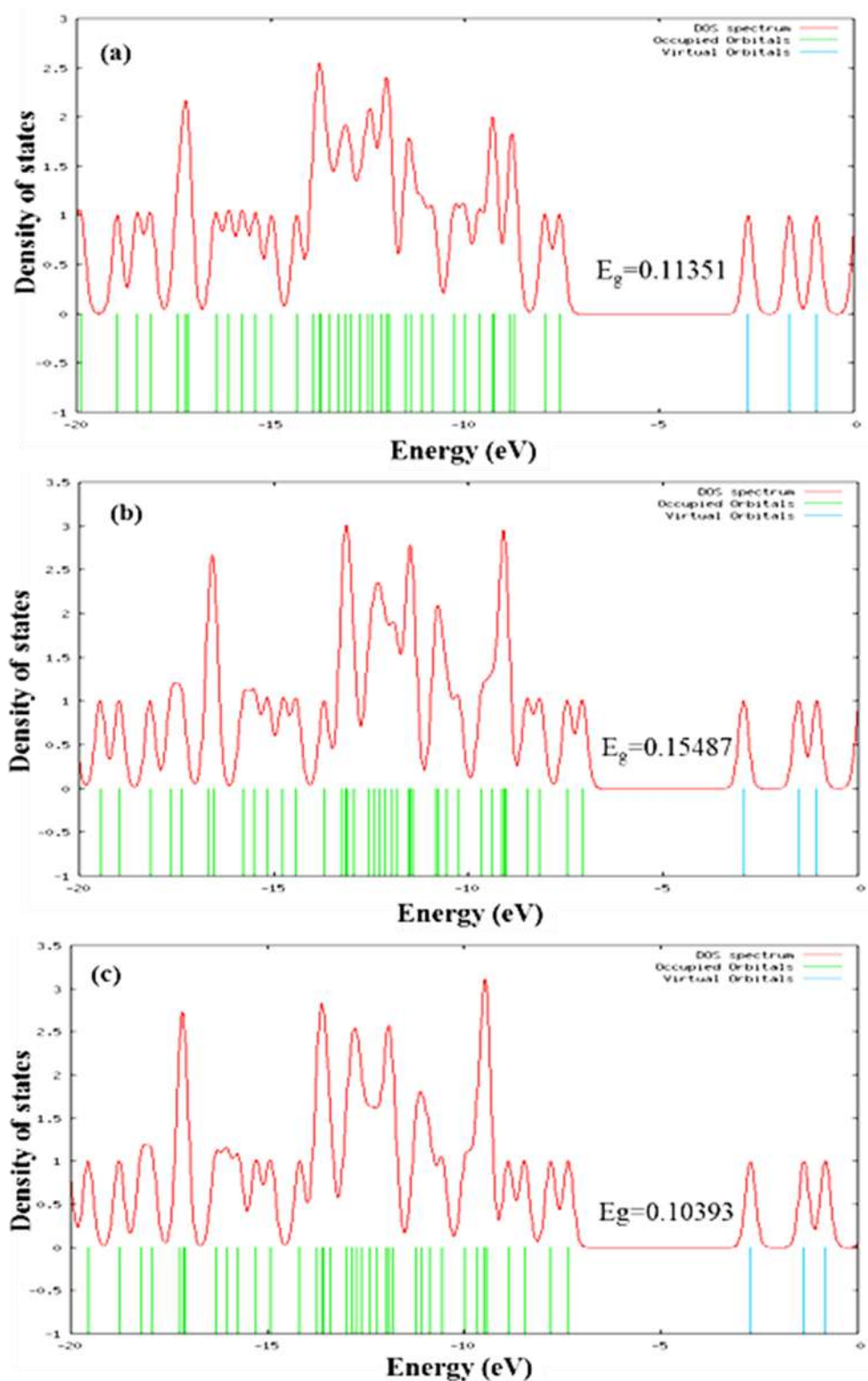
Diagram 1. An overview of the data analysis to obtain E_{HOMO} , E_{LUMO} and E_g of FLT
 Chk=C: \\ Flutamide#Opt B3LYP/6-311G (d, p)

Alpha occ. eigenvalues	--	-24.84002	-24.83611	-24.83161	-19.27624	-19.27475
Alpha occ. eigenvalues	--	-19.24459	-14.63688	-14.43206	-10.51845	-10.39039
Alpha occ. eigenvalues	--	-10.34964	-10.31939	-10.30877	-10.29685	-10.29097
Alpha occ. eigenvalues	--	-10.28966	-10.28153	-10.26265	-10.24762	-1.36926
Alpha occ. eigenvalues	--	-1.28726	-1.28179	-1.19840	-1.03671	-1.02157
Alpha occ. eigenvalues	--	-0.97576	-0.93934	-0.87571	-0.85154	-0.84002
Alpha occ. eigenvalues	--	-0.77124	-0.76321	-0.74494	-0.70069	-0.68837
Alpha occ. eigenvalues	--	-0.66409	-0.63591	-0.63249	-0.62262	-0.61171
Alpha occ. eigenvalues	--	-0.58371	-0.56729	-0.55498	-0.53586	-0.53063
Alpha occ. eigenvalues	--	-0.51610	-0.51479	-0.50749	-0.49496	-0.49081
Alpha occ. eigenvalues	--	-0.48215	-0.47750	-0.46938	-0.46669	-0.45937
Alpha occ. eigenvalues	--	-0.45302	-0.43813	-0.43766	-0.42896	-0.41519
Alpha occ. eigenvalues	--	-0.40691	-0.39784	-0.37505	-0.34737	-0.34516
Alpha occ. eigenvalues	--	-0.34223	-0.31900	-0.31095	-0.30110	-0.29732
Alpha occ. eigenvalues	--	-0.28867				
Alpha virt. eigenvalues	--	-0.17516	-0.13839	-0.06252	-0.05945	0.02943
Alpha virt. eigenvalues	--	0.04377	0.04841	0.07189	0.07762	0.08713
Alpha virt. eigenvalues	--	0.09034	0.10555	0.11620	0.12159	0.12648
Alpha virt. eigenvalues	--	0.13083	0.14026	0.14921	0.15855	0.16202
Alpha virt. eigenvalues	--	0.16517	0.16711	0.18325	0.20538	0.21124
Alpha virt. eigenvalues	--	0.21361	0.22179	0.23164	0.26015	0.26310
Alpha virt. eigenvalues	--	0.28005	0.29279	0.30016	0.32577	0.33202

Diagram 2. An overview of the data analysis to obtain E_{HOMO} , E_{LUMO} and E_g of SWCNT (5, 5)-Zn-FLT complex

Chk=C: \\ SWCNT (5, 5)-Zn-flutamide#Opt B3LYP/6-311G (d, p)

Alpha occ. eigenvalues	--	-0.37804	-0.37709	-0.37517	-0.37452	-0.37300
Alpha occ. eigenvalues	--	-0.37106	-0.37051	-0.36964	-0.36736	-0.36689
Alpha occ. eigenvalues	--	-0.36329	-0.36255	-0.36217	-0.36168	-0.35923
Alpha occ. eigenvalues	--	-0.35867	-0.35854	-0.35556	-0.35409	-0.35395
Alpha occ. eigenvalues	--	-0.35133	-0.34894	-0.34735	-0.34705	-0.34579
Alpha occ. eigenvalues	--	-0.34494	-0.34453	-0.34368	-0.34343	-0.34296
Alpha occ. eigenvalues	--	-0.34244	-0.33985	-0.33973	-0.33767	-0.33622
Alpha occ. eigenvalues	--	-0.33535	-0.33301	-0.33160	-0.32807	-0.32496
Alpha occ. eigenvalues	--	-0.32434	-0.32348	-0.32078	-0.32025	-0.31864
Alpha occ. eigenvalues	--	-0.31625	-0.31291	-0.31213	-0.31070	-0.30968
Alpha occ. eigenvalues	--	-0.30744	-0.30608	-0.30463	-0.30368	-0.30175
Alpha occ. eigenvalues	--	-0.29865	-0.28639	-0.28445	-0.28195	-0.27830
Alpha occ. eigenvalues	--	-0.27782	-0.27668	-0.27581	-0.27226	-0.27176
Alpha occ. eigenvalues	--	-0.27132	-0.26835	-0.26773	-0.26572	-0.26346
Alpha occ. eigenvalues	--	-0.26036	-0.25561	-0.25422	-0.25052	-0.24933
Alpha occ. eigenvalues	--	-0.24728	-0.24081	-0.23639	-0.23607	-0.23601
Alpha occ. eigenvalues	--	-0.23495	-0.22877	-0.22304	-0.22106	-0.21682
Alpha occ. eigenvalues	--	-0.21257	-0.21180	-0.20705	-0.19004	-0.18905
Alpha occ. eigenvalues	--	-0.18188	-0.16917	-0.16652		
Alpha virt. eigenvalues	--	-0.12799	-0.12712	-0.10725	-0.09592	-0.08720
Alpha virt. eigenvalues	--	-0.07469	-0.07309	-0.06923	-0.06781	-0.06663
Alpha virt. eigenvalues	--	-0.06453	-0.06238	-0.06074	-0.05980	-0.05817
Alpha virt. eigenvalues	--	-0.05451	-0.05431	-0.05135	-0.04994	-0.04885
Alpha virt. eigenvalues	--	-0.04261	-0.04133	-0.04020	-0.03827	-0.03620
Alpha virt. eigenvalues	--	-0.03294	-0.03015	-0.02236	-0.02119	-0.02070
Alpha virt. eigenvalues	--	-0.01705	-0.01100	-0.01035	-0.00754	-0.00539
Alpha virt. eigenvalues	--	-0.00505	-0.00192	0.00034	0.00127	0.00531
Alpha virt. eigenvalues	--	0.01266	0.01460	0.01861	0.02353	0.02424
Alpha virt. eigenvalues	--	0.02662	0.03273	0.03316	0.03328	0.03670
Alpha virt. eigenvalues	--	0.03827	0.03920	0.03960	0.04085	0.04166
Alpha virt. eigenvalues	--	0.04272	0.04725	0.05079	0.05205	0.05458
Alpha virt. eigenvalues	--	0.05827	0.05976	0.06040	0.06462	0.06926
Alpha virt. eigenvalues	--	0.07029	0.07105	0.07224	0.07484	0.07642



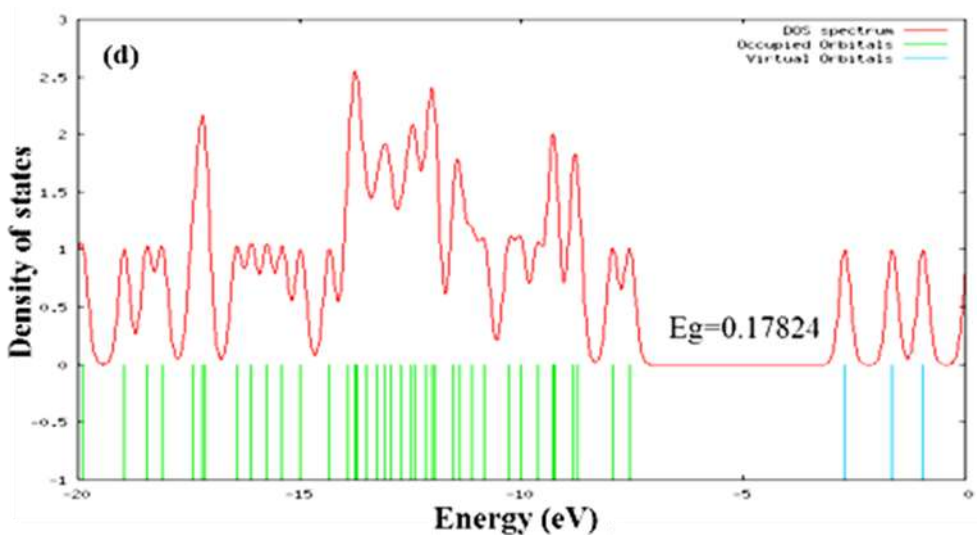


Figure 2. Orbital densities and E_g of FLT in the basis state (a) in gaseous phase, (b) in ethanol solvent, (c) in water solvent and (d) in the excited state in gaseous phase

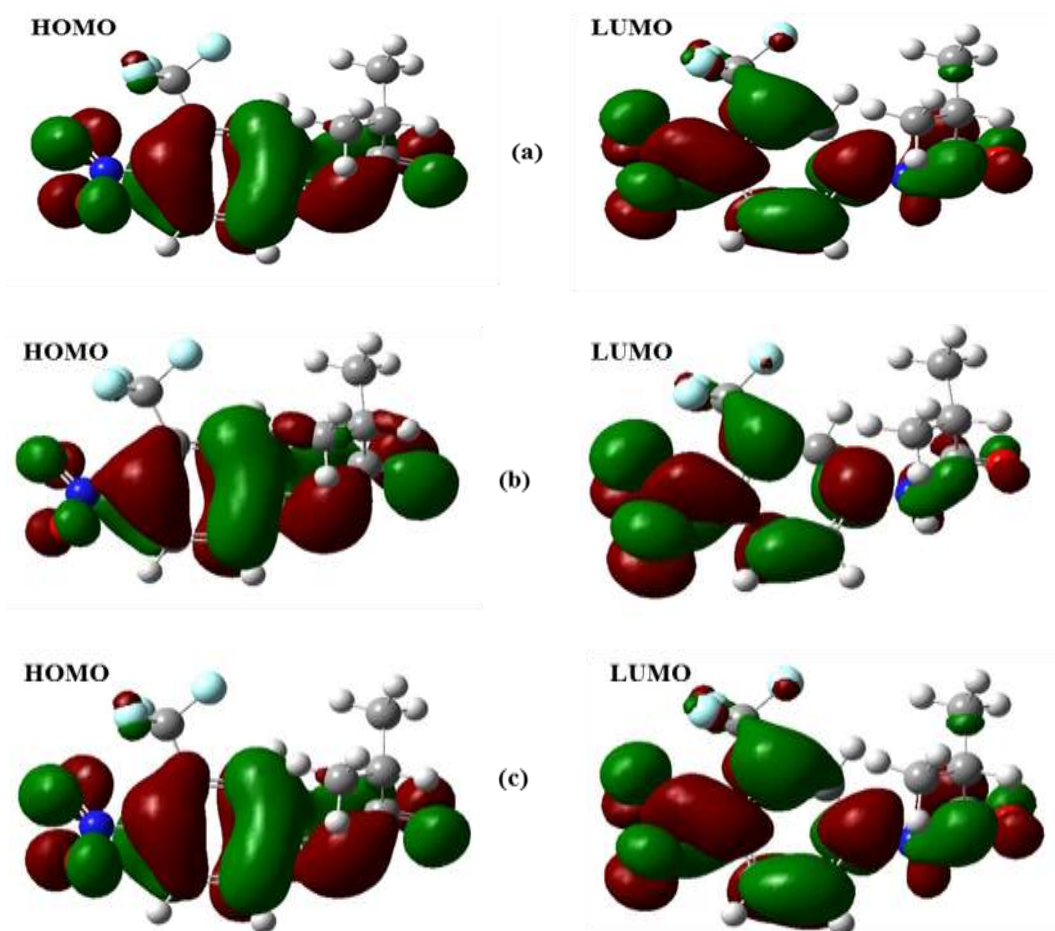


Figure 3. HOMO and LUMO orbitals of FLT in the basis state of (a) gaseous phase, (b) water solvent and (c) ethanol solvent phases

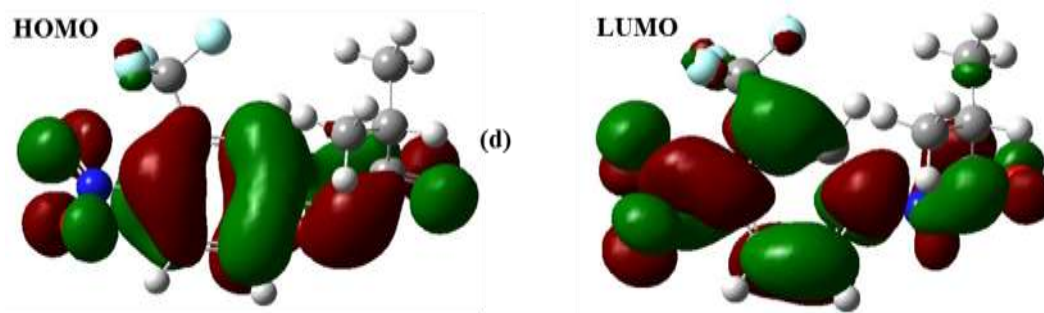


Figure 4. HOMO and LUMO orbitals of FLT (d) in the excited state in gaseous phase

Studying the interaction of FLT on the surface of SWCNT and Zn doped SWCNT

The adsorption of FLT on the surface of the pristine single-walled carbon nanotubes (SWCNT) (5, 5) and SWCNT-(5, 5)-Zn complex using DFT method at B3LYP theoretical level and at 6-311G (d, p) basis set was seriously studied. The first attempts were performed to absorb the drug over the surface of nano-tube but with no results. This can be attributed to the

repulsive force between the nanotube electron cloud and the non-bonded pair of electrons in oxygen, fluorine and nitrogen atoms in Flutamide. Afterwards, SWCNT was doped with Zn and the interaction of FLT with SWCNT- (5.5) -Zn was occurred and the SWCNT- (5.5)-Zn-FLT complex was formed. Finally, the obtained structure was optimized at B3LYP/6-311 (d, p) theoretical level (Figure 5) and then the results were extracted and studied.

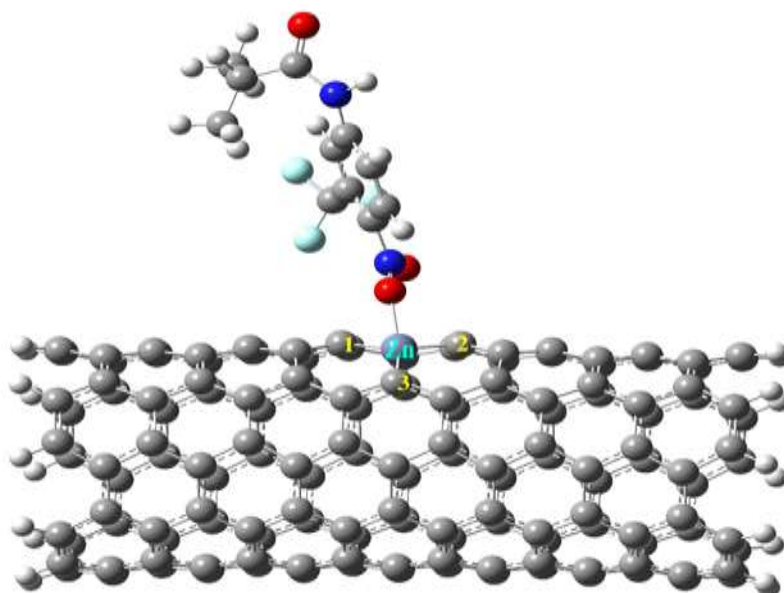


Figure 5. The optimized structure of SWCNT (5, 5)-Zn-FLT

Changes in the bond length of complex

The value of changes in bond lengths in Zn doped carbon nanotubes and the values of dipole moments after drug

absorption were calculated at B3LYP/6311(d,p) theoretical level and were reported in Table 3. Generally, if the value of the dipole moment is high,

then the absolute value of the bonding energy will increase consequently. In other words, the greater dipole moment

will lead to the noticeable increase of the excitation energy of electron clouds.

Table 3. The values of the bond length (in angstrom) and the dipole moment of drug's interaction with SWCNT (5, 5)-Zn

Complex	Dipole moment (D)	R(C ₁ -C ₂) (Å)	R(C ₂ -C ₃) (Å)	R(C ₁ -Zn) (Å)	R(C ₂ -Zn) (Å)	R(C ₃ -Zn) (Å)
SWCNT-Zn-FLT	4.0753	1.41	1.42	1.94	1.97	1.94

The adsorption energy of drug on the surface of SWCNT (5, 5)-Zn

The interaction of FLT on the outer surface of SWCNT (5, 5)-Zn was studied and the adsorption energy was calculated using Equation 2. The obtained data were reported in Table 4. As seen in Table 4, the adsorption

energy is a positive value, therefore, this interaction is endothermic and the amount of energy places it in the physisorption range. The final complex of FLT- SWCNT (5, 5)-Zn was optimized to find a stable structure (Figure 5).

$$E_{ad} = E_{tot}(FLT + SWCNT) - E_{tot}(SWCNT) - E_{tot}(FLT) \quad (2)$$

Table 4. Energy values in drug interactions on the surface of Zn doped carbon nanotube (5, 5)

Element	Energy (HF)	Energy (keV)	E _{ad} [*] (keV)
SWCNT-Zn	-7508.79	-204.33	-
FLT	-1060/43	-28.85	-
SWCNT-Zn-FLT	-8531.25	-232.15	1.033

*Calculated by equation (2)

Molecular orbital (MO) analysis of FLT- SWCNT (5, 5)-Zn

By the size reducing in semiconductor nanoparticles, the quantum effects will appear. In quantum dots, electrons also have a variety of energies, however, due to the very small size of these nanoparticles, the energy levels are not continuous. The reduction or addition in the numbers of atoms to quantum dots will cause the change in the energy gap, which undoubtedly is due to the very small size of these dots and their quantum effects. Knowing the energy

gap not only can provide the useful data about the adsorption of the molecules on the surface of nanotubes, but also make possible to study their electronic characteristics. Hence, the values of EHOMO, ELUMO and energy gap of SWCNT (5, 5), FTL and FTL- SWCNT (5, 5)-Zn in gaseous phase were also calculated using MO method and have been reported in Table 5. Considering the type of adsorption, it seems that the calculations by DFT method leads to more reasonable results.

Table 5. E_{LUMO} , E_{HOMO} , and the energy gap of the FLT on SWCNT (5, 5) -Zn

Element	E_{HOMO} (eV)	E_{LUMO} (eV)	E_g (eV)
SWCNT(5,5)	-0.15954	-0.12665	0.033
FLT	-0.27818	-0.09994	0.37812
SWCNT-Zn-FLT	-0.16652	-0.12799	0.039

Studying NMR parameters of FLT

The magnetic resonance of the nucleus (NMR), including isotropic and anisotropic chemical condensation parameters, is one of the best methods that can be used to study the electronic properties of various materials. The chemical tensors created by the positions of semi spin nuclei, C and O, not only are sensitive to the electrons, but also are easily destroyed. Therefore, they provide an important insight into the electrostatic properties of nanostructures in the drug adsorption process.

The main objective purpose in this step is to study the tendency of carbon nucleus on Zn doped SWCNT to form a physical bond with oxygen atoms of FTL (Table 6 and Figure 6). As the

charge variations on the atoms increase during the adsorption process, the molecule becomes more symmetrical and the charges of two carbons become similar and take the positive values. The reduction of the anisotropy, proves the symmetry of the electron cloud around the carbon atoms (Equations 3, 4 and 5).

$$\Delta\sigma = \frac{3}{2}(\sigma_{33} - \sigma_{iso}) \quad (3)$$

$$\sigma_{iso} = \frac{(\sigma_{11} + \sigma_{22} + \sigma_{33})}{3} \quad (4)$$

$$\eta_{\sigma} = \frac{3}{2} \left(\frac{\sigma_{22} - \sigma_{11}}{\Delta\sigma} \right) \quad (5)$$

Table 6. NMR parameters of C-O of SWCNT-Zn (5.5)-FTL

Element	Atoms	σ_{11}^a	σ_{22}^a	σ_{33}^a	σ_{iso}^a	$\Delta\sigma^a$	η_{σ}^a
FTL	C ₁	-41.5162	63.8179	66.6279	9.643	4.522	15.892
	C ₂	-29.9472	19.5015	139.0969	42.883	134.569	0.355
FTL-SWCNT-Zn	C ₁	-207.4312	23.2598	220.6322	12.153	312.717	24.199
	C ₂	-41.8461	13.7756	97.2809	97.107	111.316	14.205
	C ₃	-211.8356	174.9256	476.4464	580.760	494.901	175.370

^aCalculated σ_{ii} , σ_{iso} and $\Delta\sigma$ values are in ppm

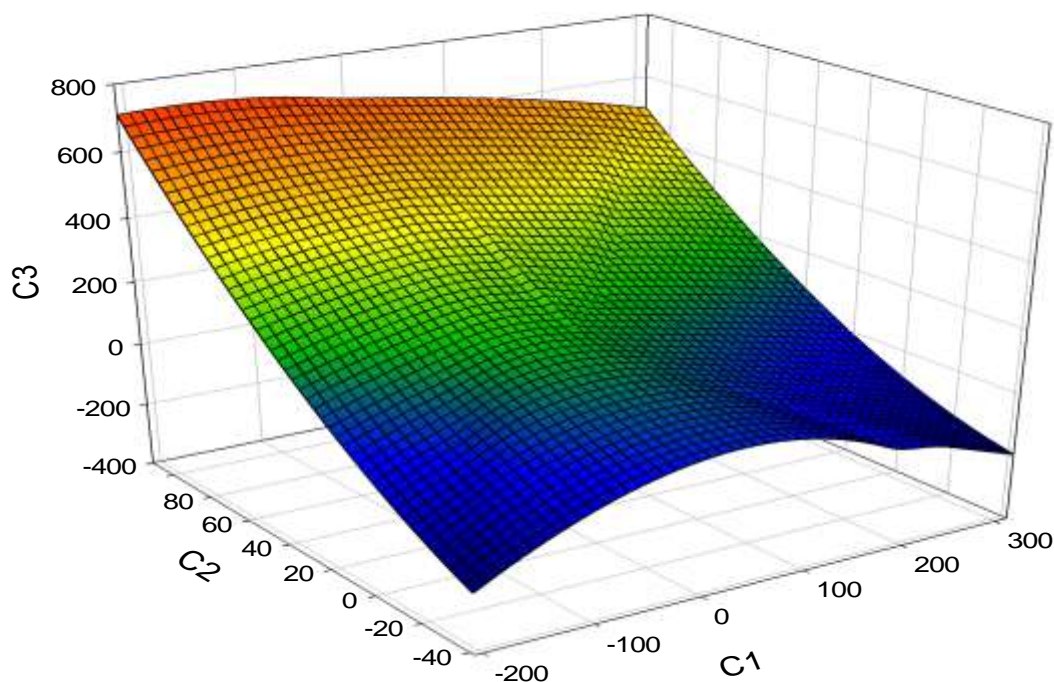


Figure 6. Variation of NMR parameters in SWCNT-Zn-FLT in C1, C2 and C3 atoms

Conclusion

In this study, the adsorption of FLT on the outer surface of SWCNT (5,5) and Zn doped SWCNT (5,5) was investigated. The carbon nanotube (5, 5) which was chosen in this study have the length of 1.73 nm and the diameter of 7.2 nm. The various structures were obtained using Gaussview software. Then, all structures were optimized properly. The optimization of these structures was carried out using the Gaussian 09 software and at B3LYP / 6-311G (d, p) theoretical level. The drug was made in both basic and excited states using DFT, and DFT-TD methods. To saturate the carbon bonds and create a model close to a real nanotube, the optimum length and diameter were assumed for calculating and finally all structures were optimized effectively. To calculate the adsorption energy, the dipole moment, the energy gap, and the values of HOMO and LUMO energies of drug

and the complex, DFT method at B3LYP / 6-311G (d, p) theoretical level and also MO method have been used. All obtained data were reported in the manuscript. The adsorption energy of FLT may be considered in the range of the physisorption. The obtained data clearly prove that the suggested SWCNT (5, 5) can be considered as the most reactive nanotube because of its small diameter and high pyramiding angle, which is an important parameter in nanotubes reactivity. Finally, it can be deduced from all the obtained data that the Zn doped nanotube (5, 5) to be interesting for drug delivery due to its relatively weak bonding.

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