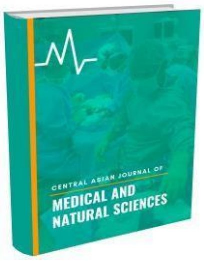

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Article

Exploring Cr, P, Al, and Si-Doped Carbon Nanotubes for Targeted Delivery of 5-Fluorouracil: Theoretical Study

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Abstract: With the use of density functional theory (DFT), the feasibility of stable interaction between a 5-fluorouracil (5-FU) drug molecule and an original carbon nanotube (CNT) doped with chrome (Cr), aluminum (Al), phosphorus (P), and silicon (Si) is examined. With its 32 carbon atoms, carbon nanotubes (CNTs) offer a convenient way to introduce many drug molecules into the body. The electrical properties of medicine fluorouracil (5-FU) as well as 5FU/metal-doped CNT are investigated with the use of the DFT approach. On the CNTs surface, metal impurities are employed to assess compatibility and maximize 5-FU adsorption. We discovered that 5-FU/metal-doped CNTs and metal-doped CNTs have different electrical band structure forms. Therefore, the electrical band gap is pushed upward and lowered (CNTS) compared to a pure CNT, yet they still exhibit semiconductor properties. Additionally, all of the complex structures gain a higher stability and become less reactive as overall energy rises. The results shown that the metal-doped CNTs and 5-FU had a stronger interaction than the pure CNTs and 5-FU. The electron affinity and chemical hardness of all structures are higher and lower, respectively. This indicates that in order for these structures to be cations or anions, they needed to donate or take a higher energy. Additionally, there is a strong connection between the original carbon nanotube (CNTS) and the 5-FU molecule in the current impurities (Cr, P, Al, and Si).

Keywords: Energy gap, total energy, CNT, 5-FU anticancer drug, Quantum chemical parameter.

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1. Introduction

Cancer is treated with the drug fluorouracil (5-FU)[1], [2], and [3]. It is used to treat a variety of cancer typess, including those of the stomach, breast, pancreas, cervix, and colon. Despite 5-FU's extensive usage in chemotherapy, its poor absorption poses a serious obstacle to its widespread application. Although significant progress was made, more investigation is still required to ascertain the most effective method of delivering 5-FU to tissues. One of the best methods for transforming such weak interactions into strong chemical bonds is doping.

Materials that may carry such medications and directly deliver them to tumors had attracted increasing interest due to their biocompatibility, biodegradability, and capacity to encapsulate certain drug molecules in their active areas [4]. Of them, CNTs' extraordinary properties have demonstrated great promise for cancer treatment. Anti-cancer drugs are not sufficiently targeted to only harm cancer cells [5].[6]. For instance, 5-FU is an anti-cancer medication because of its broad anti-tumor effect [7]. However, it contains anticancer cytotoxic drugs, which have negative side effects on the healthy as well as the cancerous cells. Reactivity and bonding features require knowledge regarding the adsorption and electrical properties of 5-FU drug on CNT surface. Thus, drug molecule adsorption had been carried out on the surface of P, Cr, Al, and Si-doped C31 in this study for determining the electrical, structural, optical, and reactivity characteristics of 5FU drug molecule as well as compare them to pristine CNT. P, Cr, Al, and Si-doped C31 have higher catalytic and reactive properties as a result of their large surface area and small size. P, Cr, Al, and Si atoms are selected as dopants because they have the lowest binding energies when compared to other atoms in the CNT models being studied [8].

In the periodic table, group atoms are located to the left of C atom and are of a lower degree of electronegativity [9], [10], and [11]. Thus, the CNT structure will have an electron-deficient area due to such dopant atoms. In this instance, the interaction between a 5FU drug molecule and the surface of CNTs (C32) and CNTs (C31W) doped was investigated using DFT/B3LYP methodologies. To our knowledge, there has never been an experimental use on P, Cr, Al, and Si-doped C31. Because of this, clinical trials for their potential applications have not yet been conducted. Hopefully, our results will direct future experimental and clinical studies.

2. Materials and Methods

The DFT is the most scalable and fundamental approach in the computational physics and chemistry. Additionally, it has shown great success in calculating the properties of ground state materials [12]. The ground state energy as well as any other ground state electronic characteristics that are solely determined through the electron density are fundamental concepts regarding the DFT. Moreover, the system's precise ground state is represented by the electronic density for low total energy [13], [14]. Using SDD basis set in this investigation, DFT was applied to the Gaussian-09 package of programs at hybrid functional B3LYP. The relativistic Effective-Core Potentials (ECPs), such the Stuttgart Dresden triple zeta ECPs (SDD) basis set, are employed for heavy metals, as in this paper. The electronic properties regarding pristine BN and BN-2X are represented by the Fermi level energy, lowest unoccupied molecular orbital (LUMO) energies, highest occupied molecular orbital (HOMO) energies, and energy gaps (i.e., difference between eigen-values of maximum valence band and minimal conduction band). (Where x stands for Ni, Cu, Fe, and Co). A mathematical expression for the energy gap can be found in [15], [16], [17], and [18]:

$$E_g = E_{LUMO} - E_{HOMO} \dots\dots\dots (1)$$

Under Koopman's approximation, the frontier orbital energies are found using the next relation [16], [19], [18], and [20].

$$\left.\begin{aligned} I.P. &= -E_{HOMO} \\ E.A. &= -E_{LUMO} \end{aligned}\right\} \dots\dots\dots\dots (2)$$

The values of electron affinity (E.A.) and ionization potential (I.P.) could then be utilized in order to calculate electro-negativity, softness, hardness, and electrophilicity. DFT was widely used to predict molecular properties regarding structure. This theory describes key reactivity indices as electronic energy (E) derivatives with respect to number of electrons (N) with constant external potential $\upsilon(r)$. These indices include electronegativity (χ), softness (σ), chemical hardness (η), and electrophilicity (ω). These notions include the next quantitative expressions [19], [21], [22], and [23]:

$$\boldsymbol{\chi = \frac{I.P.+E.A.}{2} \dots\dots\dots\dots\dots (3)}$$

$$\boldsymbol{\eta = \frac{I.P.-E.A.}{2} \dots\dots\dots\dots\dots (4)}$$

$$\boldsymbol{\sigma = \frac{1}{2\eta} \dots\dots\dots\dots\dots\dots\dots\dots (5)}$$

$$\boldsymbol{\omega = \frac{(I.P.+E.A.)^2}{4(I.P.-E.A.)} \dots\dots\dots\dots\dots (6)}$$

Adsorption distance (d) was computed in order to evaluate adsorption parameters, like the adsorbent strength between Bilayer BN and gas atom energy. The definition of adsorption energy is as follows [24], [25], and [26]:

$$E_{ad} = E_{BN\text{-}GAS} - E_{BN} - E_{gas} \text{ .... } \mathbf{(7)}$$

3. Results and Discussion

DFT computations are used for optimizing the geometrical structures regarding anticancer drugs. Here, by calculating the adsorption interaction between pristine CNT and various anticancer drugs, we looked into how pristine CNT might be used as a carrier for anticancer medications. The anticancer medications 5-FU, CNTs-pristine, and 5-FU-CNTs-pristine are shown in Figure 1.

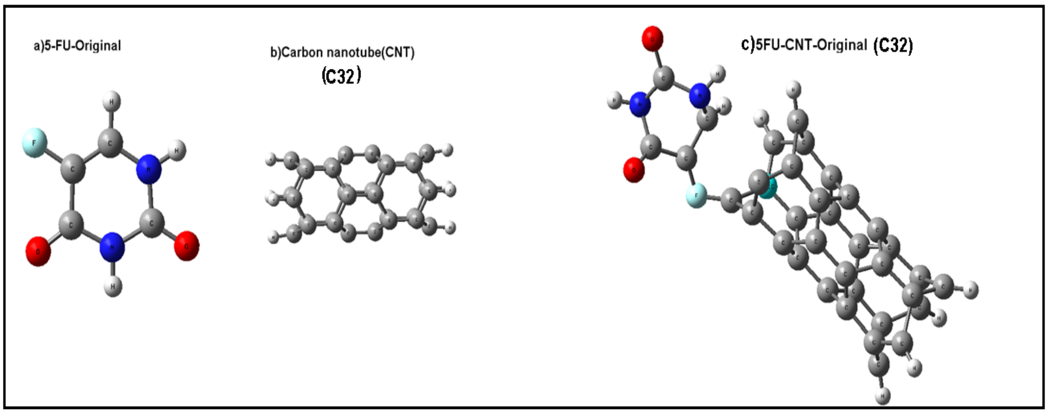

Fig.1: Optimization geometry of the a)5-FU, b) pristine -CNT- and c) 5-FU- pristine -CNT

In figure 2 represents optimization geometry of the metal-doped-CNT31-W, where the carbon atom

has been replaced with a W atom (where W=Al, Cr, Si and P). The covalent nature of anti-cancer drug and pristine CNT was demonstrated by 1.3–1.7Å distance between the anticancer drug and CNT surface. Through calculating total energy, which equals the summation of electrostatic, kinetic, and exchange-correlation energies, we may investigate the metal-doped CNT structures' stability. Boost the metal-doped CNT's overall energy in comparison to the pristine CNT. The metal-doped CNT structures are hence getting more stable. Furthermore, it was shown that all of the metal-doped CNT structures had reduced electronic band gap with direct transition, exhibiting semiconductor behaviors with minimal changes in the electronic band gap regarding such complex structures. As summarized in Table 1, we found that CNT-Si had the lowest energy gap when put to comparison with the other structures. Furthermore, in contrast to the pristine examples, Fermi level is moved up to conduction band of all the complicated structures. Through optimizing the geometrical structure as well as computing the values regarding the HOMO, LUMO, energy gap, total, and adsorption energies, we examined the stability of 5FU/pristine-CNT and 5-FU/metal-doped CNT31-W structures. Results are summarized in Table 1. According to the frequency computations, the virial ratio (-V/T) values fall between 2.0035-2.0048, and the results reveal a decent relaxation with no imaginary frequencies.

Table 1. The values of energy of the HOMO and LUMO, band gap (Egap) and adsorption energy (Eads) estimated for the 5-FU and pristine and metal-doped CNT

All properties in e V				
System	HOMO	LUMO	Energy gap	Total energy
5-FU	-7.097	-1.7950	5.302	-13982.81
Pristine-CNT	-5.387	-3.1666	2.220	-33108.635
Cr-CNT	-5.283	-3.3593	1.924	-60626.86
P-CNT	-5.464	-3.6850	1.779	-38789.348
Al-CNT	-5.405	-3.6755	1.729	-40087.715
Si-CNT	-5.486	-4.0001	1.486	-41481.412

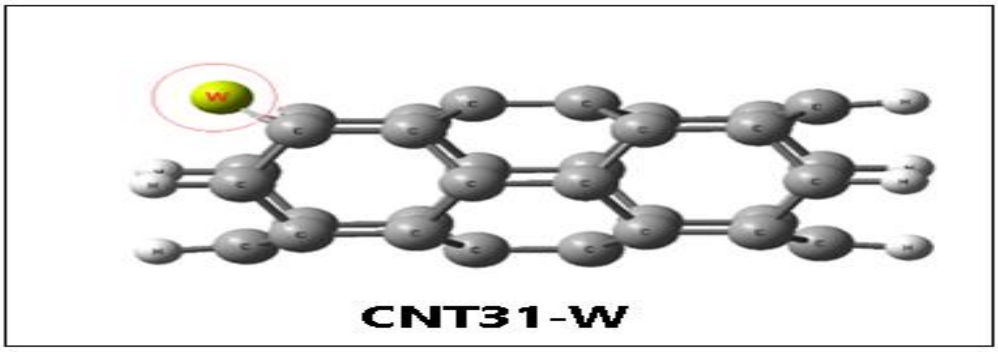

Fig2: Optimization geometry of metal-doped Carbon nanotube, where W=Al, Cr, Si and P

The 5-FU drug molecule-metal-doped C31-W's optimized geometry, in which W stands for Al, Cr, Si, and P. The electronic characteristics of 5FU/metal-doped CNT were calculated. With the use of impurities of Al, Cr, Si, and P. Refer to Table 2. We discovered that there is a change in the format of the electronic band structure between 5-FU and such impurities. As a result, 5-FU/metal-doped CNT structures' electronic band gap drops from 1.82eV for 5-FU/CNT-P to 1.49 eV for 5-FU-CNT-Si. Therefore, following W-doping, the LUMO and HOMO levels are not sanitized, which is significant for drug delivery systems and shows that the doping procedure is relatively safe from an electronic standpoint. Semiconductor characteristics are still present in such structures. as listed in Table3. The stability of 5FU/metal-doped CNT structures was also computed. Because the total energy is higher, all of such structures are less reactive and more stable. The results above indicate that we could deliver a 5FU drug molecule using pristine and metal-doped CNT as a membrane.

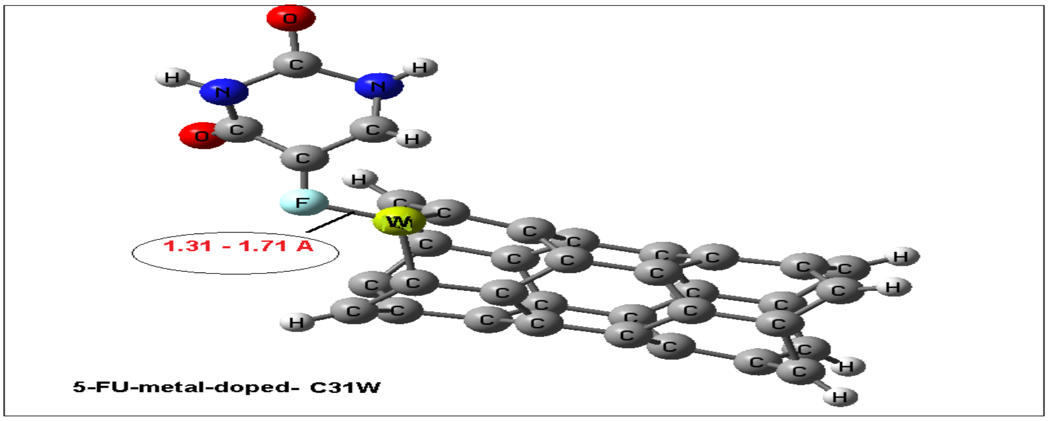

Fig.3: Optimized geometry of 5FU-metal-doped C31-W, where W=Al, Cr, Si and P

Table 2: The values the energies of HOMO and LUMO, band gap (Egap) and adsorption energy (Eads) that had been calculated for 5FU-CNT and 5FU-CNT31W

System	**HOMO**	**LUMO**	**Energy gap**	**total energy (a.u)**	Adsorption energy **(eV)**
5-FU-CNT	-5.926	-4.101	1.824	-47239.467	4.77
5-FU--Cr-CNT	-5.487	-3.913	1.574	-74611.348	0.05
5-FU-Al-CNT	-5.333	-3.735	1.598	-52772.584	0.01
5-FU-Si-CNT	-4.699	-3.203	1.496	-54071.315	0.02
5-FU-P-CNT	-5.190	-3.372	1.818	-55482.025	0.57

In table 2, the values of hardness and softness were calculated because they represent part of the important properties. we noted the hardness is a small value for the pristine -CNT, which describes this structure has a higher capability for transferring an electron. Then, it can be seen that the highest value of hardness is corresponding to the lowest softness value and vice versa. For example, the hardness value of5-FU-pristine- CNT compound is equal to (0.91eV), which is the lowest value in Table (3) Which corresponds to the lowest value of softness which equals (0.54eV). This result confirms the previous statement, where hardness and softness are considered a function of the energy gap, that is, the lowest value of the energy gap agrees with the lowest value of the hardness parameter. Therefore, the FU-CNT-Si compound are the best structures, and this is due to the few hardness value that the compound possesses and which makes the compound very important as drug delivery. for softness, there is a larger separation between valence and conduction bands due to the value of the **S** is a smaller for the pristine CNT and complex structures 5-FU/pristine CNT and CNT31-W.

The complex structures 5-FU/pristine CNT and CNT31-W have IP greater than the EA. Therefore, the higher value of the IP means that the structure is difficult tendency to donating an electron. So, pristine -CNT has a higher value of the IP, which refers to that it needs higher energy to donating an electron in comparison with other structures, which under study. For EA, the pristine -CNT and all complex structures have a smaller value, which means that these structures have lower ability to accepting an electron. it has high ability to accepting electrons.

Table 3: The values of electron affinity (EA), chemical hardness (H), electronegativity (EN), ionization potential (IP), chemical potential (μ), chemical softness (S), and electrophilic (ω) calculated for all structures.

System	Hardness	Softness	Ionization	Electron affinity(eV)
Pristine-CNT	1.110168	0.45038228	5.3870358	0.11638
5FU	2.651342	0.18858372	7.0977285	1.7950437
5-FU-CNT	0.912487	0.5479528	5.9260659	4.1010912
5-FU-Cr-CNT	0.787185	0.63517446	5.4874407	3.9130701
5-FU-Al-CNT	0.799294	0.62555225	5.3337042	3.7351167
5-FU-Si-CNT	0.748411	0.66808207	4.6999833	3.2031612
5-FU-P-CNT	0.909086	0.55000291	5.19098775	3.37281555

4. Conclusion

The electrical structures and geometries of a 5-fluorouracil drug molecule were studied using the SDD/B3LYP-DFT interaction with an original carbon nanotube (CNT) doped with silicon (Si), aluminum (Al), phosphorus (P), and chrome. The distance between the clean CNT surface and these anticancer medicines is 1.3-1.7Å. The electrical band gap of 5-FU/metal-doped CNT structures is reduced from 1.82eV for 5-FU/CNT-P to 1.49eV for 5-FU-CNT-Si. Thus, the HOMO and LUMO levels are unsterilized following the W-doping, which is critical for the drug delivery systems. pure -CNT has a greater value of the IP, which alludes to the fact that it requires more energy to donate an electron in contrast to other structures under examination.

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