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Density Functional Theory Study of the Behavior of Carbon Nano cone, BP Nano cone and CSi Nano cone as Nano Carriers for 5-Fluorouracil Anticancer Drug in Water

Tahereh sadat Nasiri Moghaddam, Farrokh Roya Nikmaram*, Roya Ahmadi

Department of Chemistry, Faculty of Science, Yadegar-e-Imam Khomeini (RAH) Shahre Rey Branch, Islamic Azad University, Tehran, Iran

*. *e-mail: nikmaram87@yahoo.com*

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Abstract

In this work, the electronic properties of BP and CSi Nano cones have been investigated by self-consistent reaction field (SCRF) method in water solvent at B3PW91/6-31G (d,p) level of DFT theory for study of for interactions of 5-Fluorouracil Anticancer Drug with theses Nano cones. The percent of change of energy gap ($\%\Delta E_g$) shows that the complex formation of 5-Fluorouracil with BP nano cone is more suitable.

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Keywords: BP Nano cone, CSi Nano cone, 5-Fluorouracil, Nano Carrier, Solvent, DFT

1. Introduction

Fluorouracil is an anticancer drug as intercepter of cancer cells activities [1-3]. The role of carbon nanotubes as drug delivery of 5- -Fluorouracil Anticancer Drug are said at different researches [4-6].

The Nano cones are the type of nano materials that observed as caps on the ends of nanotubes, and also as free standing nanostructures, Fig.1. [7]. More recently, a theoretical study by Alfieri and Kimoto have indicated that Nano cones with disclination angles 60º ,120º, 240ºand 300ºare stable[8]. The cone is entirely characterized by its cone angle [9]. Carbon cones have also been observed, since 1968 or even earlier on the surface of naturally occurring graphite [10]. Carbon Nano cones are produced in an industrial process that decomposes hydrocarbons into carbon and hydrogen with a plasma torch having a plasma temperature above 2000 °C [11]. A comparative research on the role of carbon nanotube and Calix arene as drug delivery of 5-Fluorouracil Anticancer Drugs show that the complex of p-Sulphonatocalix [4] arene and Fluorouracil is more stable than nanotube-Fluorouracil due to the large energy gap [6]. Therefore, the study of electronic properties of nanostructures is important for investigation of complex formation. The electronic properties have been described by Natural Bond Orbital (NBO) analysis [12].

2. Computational details

In our work, the interaction of 5-Fluorouracil (5-FU) with Carbon nano cone, BP Nano cone and CSi Nano cone were studied by self-consistent reaction field (SCRF) method in water solvent at B3PW91 level of DFT with 6-31G(d,p) basis set. A small cluster of nano cone with disclination angle equal to 240º and height equal to 4 have been created by Nanotube Modeler 2014 software [13].

The interaction energies (ΔE_{int}) of studied complex systems have been obtained by Eq.1.

$$\Delta E_{int} = E_{complex} - (E_{Nano\ cone} + E_{5-Fluorouracil}) \qquad Eq.1$$

The first term in Eq.1 is the energy of the complex system and the next two terms are the energies of the free Nano cone molecule and bare 5-Fluorouracil, respectively.

The harmonic vibrational frequencies of the fully optimized structures have been calculated to confirm the stationary point as a local minima with all positive frequencies. The electronic properties of nanostructures have been described by lowest unoccupied molecular orbital (LUMO) and highest occupied molecular orbital (HOMO).

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3. RESULTS AND DISCUSSION

The structural stability of nanostructures can be described by calculated energy. In this work, the interaction between 5-FU and Nano cone has been studied for Fluorine position of connection. Table 1 presents the dipole moments, interaction energies (ΔE_{int}), Gap of Energy (E_g) and $\%\Delta E_g$ for all the interacting systems. The values of ΔE_{int} show that the connection between the Fluorine atom of 5-FU with Phosphorus of BP Nano cone (-137.4862 kcal.mol^{-1}) is energetically favored over other complexes.

Also, the gap of energy of 5-FU, BP nano cone complex (P…F) decrease with respect to single nano cone. The calculated %ΔEg for 5-FU, BP nano cone complex (P…F) is -82.31. The E_{gap} of 5-FU, BP nano cone complex (P…F) has distinctively changed from 2.1651 to 0.3829 by -82.31% change.

Dipole moment gives clear information about the arrangement of charges in nanostructures. The result of dipole moment may indicate that the type effect of atom is important and asymmetry in charge distribution in nanocones can further be explained to achieve different electronic properties. At all of the structures, the dipole moment of connected structures are increased.

The electron resonance (E^2) at Table 2 is a factor of electron mobility. Thus, the narrow band gap (0.3829 eV) between the HOMO and LUMO levels for 5-FU, BP nano cone complex (P…F) results in easy transition of electrons from HOMO level to LUMO and easy mobility of electrons (E^2=54.05) at this complex. This means that the 5-FU drug molecule is coupled to the BP nano cone that have effected on the electronic charge distribution of atoms of nano cone, so, considerable charge transfer takes place between the drug molecule and nano cone.

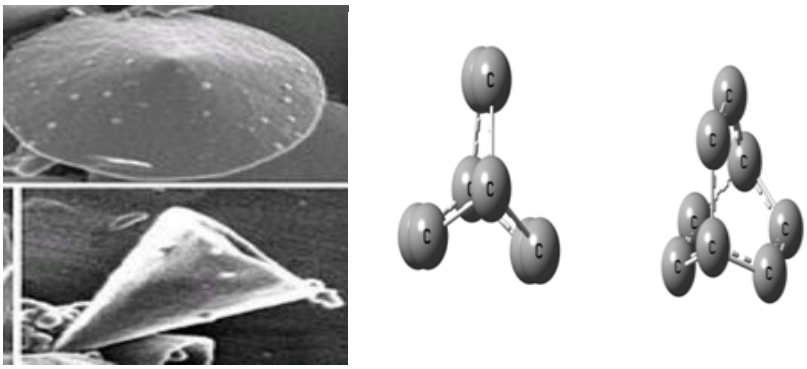

Fig1: Carbon nano cone from three view

Table1: Gap of Energy (E_g) and $\%\Delta E_g$ in water at B3PW91/6-31G(d,p)				
structure	μ/ Debye (Δμ)	E/ a.u (ΔE_{int} /kcal.mol^{-1})	E $_g$ /eV	$\%\Delta E_g$
5-Fluoro Uracil	6.2267	-527.140	6.1878261	-
Carbon nanocone	0.0002	-318.0543	9.33303	-
5-FU, Carbon nano cone complex (F…C)	11.1384 (4.9115)	-836.798 (-54.3221)	4.6349514	50.33
BP nanocone	4.451	-336.1221	2.1651	-
5-FU, BP nano cone complex (B…F)	11.5176 (0.8399)	-832.203 (-120.204)	0.824735	-61.90
5-FU, BP nano cone complex (P…F)	12.4067 (1.729)	-833.176 (-137.4862)	0.3829	-82.31
CSi nanocone	1.9096	-328.0929	3.8809623	-
5-FU, CSi nano cone complex (F…C)	12.3616 (4.2253)	-874.4330 (-104.5527)	2.63937	-31.99
5-FU, CSi nano cone complex (F…Si)	20.5624 (12.4261)	-857.0052 (-113.2011)	2.5634541	-33.94

Table2: NBO Analysis in water at B3PW91/6-31G(d,p)							
Donor NBO (i)	Acceptor NBO (j)	E^2 (kcal/mol)	q	Occupancy (i)	Energy (i)	Occupancy (j)	Energy (i)
5-FU, Carbon nano cone complex							
BD (1) C14 - C16 C14: SP 2.95 C16: SP 2.31	BD*(1) C – F C: SP 2.53 O: SP 5.69	40.60	0.058	1.6269	-0.7708	0.2180	0.1611
5-FU, BP nano cone complex							
BD (1) C14 - C16 C14: SP 2.01 C16: SP 2.41	BD*(1) C - F C: SP 3.20 F: SP 3.81	54.05	0.286	1.6921	-0.5660	0.1177	0.1533
5-FU, CSi nano cone complex							

BD (1)C14 – F C14: $SP^{2.07}$ F: $SP^{2.48}$	BD*(1) F - Si F:SP2.29 Si: SP 7.08	44.78	0.193	1.5430	-0.4120	0.1109	0.1411

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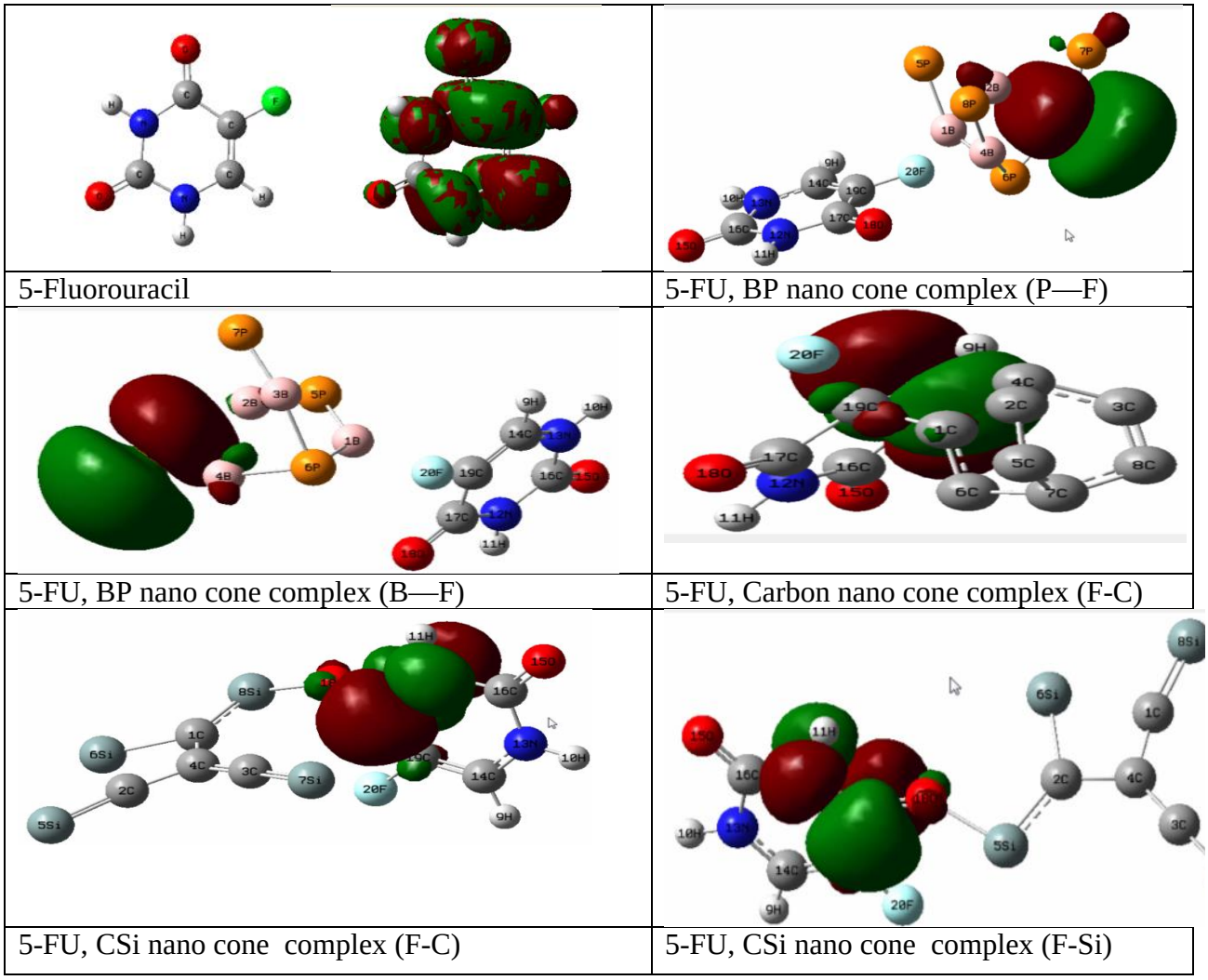

Fig2. The most stable complexes and Lumo and Homo orbitals at B3PW91/6-31G (d,p) level

4. Conclusions

We are finding the BP nano cone is more sensitive for complex formation with 5-FU drug with the decrease in the energy gap (%ΔE_g = -82.31eV) in comparison with other complexes. This finding reveals that the 5-FU molecule has stronger actions with BP nanocone.

5. References:

[1]. Dorr, RT, Von-Hoff, DD: Cancer Chemotherapy Handbook, 2nd edn, pp. 27–28. Appleton and Lange, Norwalk (1994).
[2]. Chu, E: Clinical colorectal cancer: ode to 5-fluorouracil. Clin. Colorectal Cancer 6(9), 609 (2007).
[3]. Longley, DB, Harkin, DP, Johnston, PG: 5-fluorouracil: mechanisms of action and clinical strategies. Nat. Rev. Cancer 3(5), 330–338 (May 2003).
[4]. Dresselhaus, MS, Dresselhaus, G, Eklund, PC: Science of Fullerenes and Carbon Nanotubes. Academic Press, San Diego (1996).
[5]. Kong, J, Franklin, NR, Zhou, C, Chapline, M, Peng, G, Cho, SK, Dai, H:Nanotube molecular wires as chemical sensors. Science 287, 622–625 (2000).
[6. Comparison of drug delivery systems: Nanotube and p- Sulphonatocalix[4]arene, by Density Functional Theory, Zare and Shadmani Journal Of Nanostructure in Chemistry 2013, 2013, 3:72.
[7]. S. Iijima, T. Ichihashi, Y. Ando, Pentagons, heptagons and negative curvature in graphite microtubule growth. Nature. 356 (1992) 776–778.
[8]. G. Alfieri, T. Kimoto, Structural stability and electronic properties of SiC nanocones: first-principles calculations and symmetry considerations, Appl Phys Lett. 98 (2011) 123102.
[9]. M. Ge and K. Sattler, Observation of fullerene cones, Chem. Phys. Lett. 220 (1994) 192-196.
[10]. Gillot, J; Bollmann, W; Lux, B (1968). "181. Cigar-shaped conical crystals of graphite". Carbon 6 (2): 237.
[11]. Naess, Stine Nalum; Elgsaeter, Arnljot; Helgesen, Geir; Knudsen, Kenneth D (2009). "Carbon nanocones: wall structure and morphology". Science and Technology of Advanced Materials 10 (6).
[12]. V. Nagarajan, R. Chandiramouli, S. Sriram , P. Gopinath, Quantum chemical studies on the structural and electronic properties of nickel sulphide and iron sulphide nanoclusters, J Nanostruct Chem. 4 (2014) 87-102.
[13]. Nanotube Modeler JCrystal Soft, 2014 software.