American Journal of Materials Science 2017, 7(1): 12-17
DOI: 10.5923/j.materials.20170701.02

Structural and Electronic Properties of InGaP Nanocrystal Diamantane Drug Carrier

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Abstract Nanotechnology is being applied to improve drug delivery in a number of ways. One of these ways is via built drug carriers. Nanosized particles of drug carriers are optimized for absorption of drugs through inhalation therapy. Modeling and simulation of nanocrystal parameters of the 5-Fluorouracil with indium gallium phosphide in diamantane structure have been performed with Gaussian 09 program. Density functional theory has been used for $In_5Ga_2P_7$ nanocrystal, 5-Fluorouracil drug. Optimization plus frequency at the ground state level, PBEPBE, 3-21G basis sets has been investigated. The charges for all are equal to zero charges. Molecular orbital theory has been used to find highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies. Total energy, ionization potential and electron affinity have been calculated for $In_5Ga_2P_7$ nanocrystal with 5-Fluorouracil drug.

Keywords Modeling, Simulation, Diamantane, Drug carrier, Density functional theory, and nanocrystal

1. Introduction

The number of products based on new drug delivery systems has significantly increased in the past few years, and this growth is expected to continue in the near future. Recent advances in the field of genomics have accelerated research of biopharmaceuticals, and today a large number of companies are busy developing protein- and peptide-based drugs [1]. These biopharmaceuticals present challenges to drug delivery scientists because of their unique nature and difficulty in delivery through conventional routes [2].

Fluorouracil (5-FU) is medication drug used in cancer treatment. It is a suicide inhibitor and works through irreversible inhibition of thymidylate synthase. It belongs to the family of drugs called the antimetabolites [3]. It is on the World Health Organization's List of Essential Medicines, the most important medications needed in a basic health system [4]. Antimetabolite drugs work by inhibiting essential biosynthetic processes, or by being incorporated into macromolecules, such as DNA and RNA, and inhibiting their normal function. The fluoropyrimidine 5-fluorouracil (5-FU) does both [5].

Nanoparticles are especially adaptable for delivery non – soluble and hydrophobic drugs. The size domain of particles between 10 and 100 nm lies between the size of materials that are extracted from the blood by microtubule filtration in the kidneys, and the sizes that are trapped by the liver, gall bladder, and liver, or that block capillaries in the lungs or other organs to cause emboli. If the dimensions of nanocrystal are smaller than twice the Bohr radius of the material it is made of, then quantum confinement occurs [6].

For the treatment of human diseases, nasal and pulmonary routes of drug delivery are gaining increasing importance [7]. The aim of this work is modeling and simulation to the creation and design of nanocrystal material of gallium indium phosphide which can be used for drug carrier to the place of destination in the human body using diamantane structure.

2. Materials and Methods

Geometry optimization is name for the procedure that attempt to find the configuration of minimum energy of the molecule [8]. The procedure calculates the wave function and the energy at starting geometry and then proceeds to search a new geometry of a lower energy [9]. This is repeated until the lowest energy geometry is found the procedure calculates the force on each atom by evaluating the gradient (first derivative) of the energy with respect to atomic positions sophisticated algorithms are then used at each step to select a new geometry [10].

Diamondoids have been of great interest in recent years due to their role in nanotechnology, drug-delivery and medicine. The carbon-carbon framework of diamondoids constitutes the fundamental repeating unit in the diamond lattice structure. It is demonstrated that diamondoids are very stable compound [11, 12].

The smaller diamondoid molecules, with the general chemical formula $C_{4n+6}H_{4n+12}$: adamantane ($C_{10}H_{16}$),

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Published online at http://journal.sapub.org/materials

diamantane ($C_{14}H_{20}$), and tiramantane ($C_{18}H_{24}$). Each of these three lower adamantologues has only one isomer [13].

DFT is a computational quantum mechanical modeling method used in physics, chemistry and material science to investigate the electronic structure (principally the ground state) of many body systems, in particular atoms, molecules and condensed phases [14, 15]. With this theory the properties of a many electron system can be determined by using functional i.e. functions of another function which in this case is the spatially dependent electron density [16]. Hence the name density functional theory comes from the use of functional of the electron density [17].

Indium Gallium phosphide (InGaP) is a semiconductor composed of indium, gallium and phosphorus. The $In_XGa_{1-X}P$ ternary alloy is an attractive material for the preparation of variety of optoelectronic and microelectronic devices. The band gap energy is usually determined using a parabolic interpolation between (GaP) and (InP) [18].

Theophylline is used to prevent and treat wheezing, shortness of breath, and chest tightness caused by asthma, chronic bronchitis, emphysema, and other lung diseases. It relaxes and opens air passages in the lungs, making it easier to breathe [19]. DFT partition the total energy as [20, 21]:

$$E = E_T + E_v + E_J + E_{XC} \quad (1)$$

where E_T: Electronic kinetic energy, E_v: Electronuclear interaction energy, E_J: Electron-electron repulsion, and E_{XC}: Exchange correlation term.

According to Koopman's theorm in which the frontier orbital energies are given as [23]:

$$E_{HOMO} = -I.P \quad (2)$$

$$E_{LUMO} = -E.A \quad (3)$$

$I.P$, ionization potential and $E.A$, electron affinity.

For the equilibrium system (e.g. atoms or molecules), let E(N) represent a ground state electronic energy as a function of the number of electrons (N). It is well-known the derivative of $E(N)$ with respect to (N) at a constant external potential, $V(\vec{r})$, the chemical potential (κ) or the electronegativity (χ) of the absolute negativity are [24]:

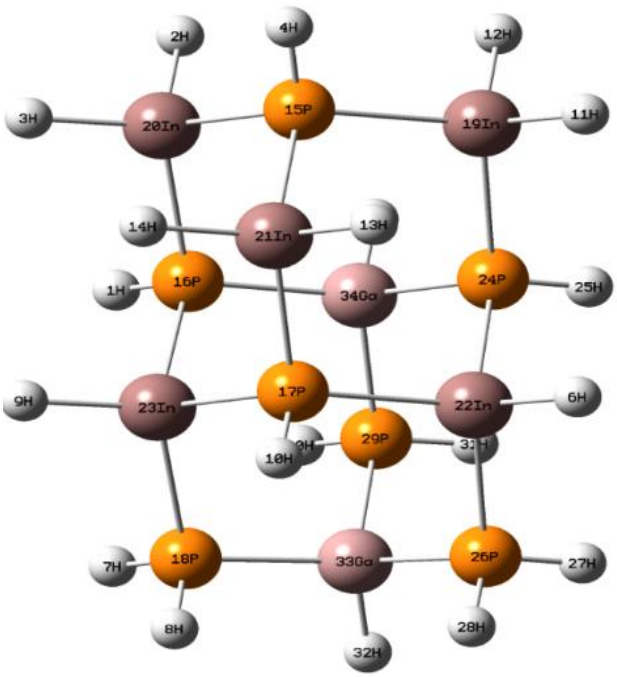
$$\kappa \approx -\chi = -\frac{(IP+EA)}{2} \quad (4)$$

The theoretical definition of chemical hardness (η) has been provided by the density functional theory as the second derivative of electronic energy with respect to the number of electrons N at a constant external potential $V(\vec{r})$ [25]

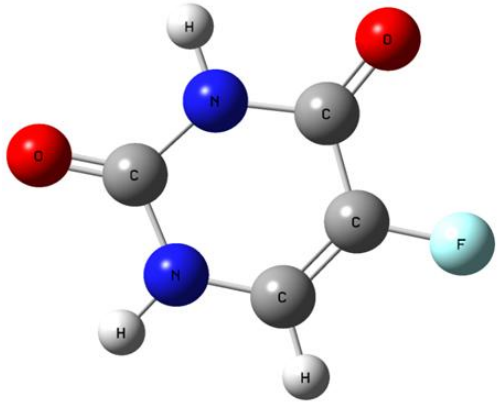
$$\eta = \frac{(IP-EA)}{2} \quad (5)$$

Equation (5) shows that chemical hardness is the resistance of the chemical potential to change in the number of electrons of the highest occupied and lowest unoccupied molecular orbital (HOMO and the LUMO energies) of the neutral molecule and is known as orbital-vertical [26, 27].

All the computational studies were carried out using the density functional theory (DFT) implemented in the Gaussian 09W suite of programs. 27 Gaussian, a commercial quantum chemical software package from Gaussian incorporation is considered to be the industry standard in the area of molecular modeling and computational chemistry.



$In_5Ga_2P_7$



5Fluorouracil ($C_4H_3FN_2O_2$)

Figure (1). The optimized structure of InGaP diamantane nanocrystal and 5Fluorouracil with PBEPBE/3-21 G method

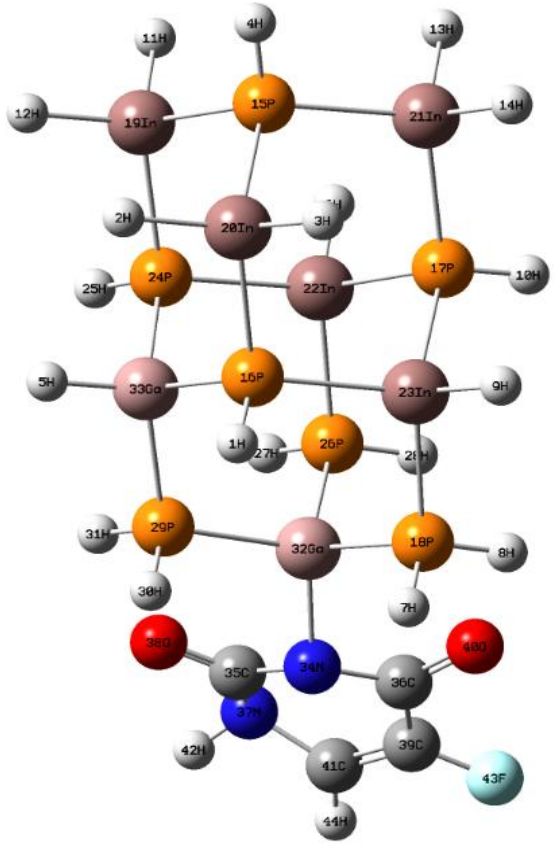


Figure (2). Optimized structure of InGaP diamantane nanocrystal with PBEPBE/3-21 G method

Gaussian is capable of running all of the major methods in molecular modeling, including molecular mechanics; *Ab*-initio; semi empirical, and density functional theory (DFT). The molecular properties of the compounds have been computed by DFT using the standard 3-21G basis set. In the DFT calculations the Lee, Yang and Parr correlation functional is used together with Becke's three parameters exchange functional B3LYP. Conformational analysis of the molecules has been performed to have an idea about the lowest energy structures of the species.

3. Results and Discussion

The optimization structure for $In_5Ga_2P_7$ diamantane nanocrystal was calculated by using Gaussian 09 program. Figure (1) can be shown that the geometric structure of InGaP diamantane nanocrystal, 5Fluorouracil ($C_4H_3FN_2O_2$) and the number of atoms, so that these atoms in the molecule are numbered according to their order in the molecule specification section of the input. Figure (2) shows the optimized structure of 5-Fluorouraci-$In_5Ga_2P_7$ Diamantane with PBEPBE/3-21G method.

Table (1) represents the total energy for $In_5Ga_2P_7$ diamantane, 5-fluorouracil drug and $In_5Ga_2P_7$ diamantane binding 5-Fluorouracil. The total energy for $In_5Ga_2P_7$ diamantane binding 5-Fluorouracil is less than the total energy for $In_5Ga_2P_7$ diamantane, shown that the total energy decreases with increasing the number of Ga atoms using PBEPBE/3-21G (basis sets).

Table (1). Total energy, HOMO, LUMO, and energy gap for InGaP nanocrystal and drug –InGaP. nanocrystal

Properties	InGaP	5Fluorouracil	InGaP - 5Fluorouracil
Total energy, MeV	-0.947047	-0.01389	-0.960913
E_{HOMO}, MeV	-5.649	-5.619	-5.578
E_{LUMO}, MeV	-1.937	-1.902	-2.88
E_{Gap}, MeV	3.683	3.717	2.6693

The size dependence of the energy is linear inversely proportional. Note that the total energy decreases with increasing the number of atoms in the diamantane structure, can be explained based on the principle of Heisenberg as the outer electrons of each atom in the system spend more time in region between atoms bound according Coulomb law, so it is more stable compound for drug delivery.

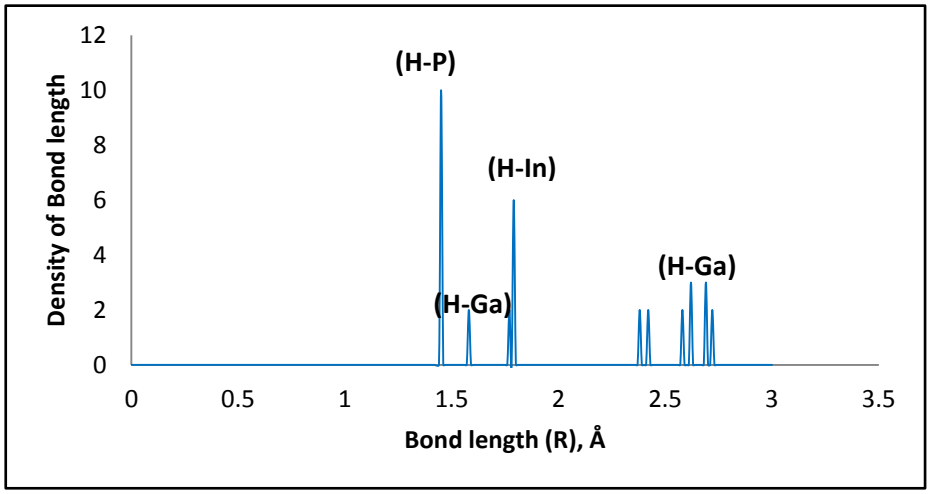


Figure (3). Distribution of Bond lengths (R) in InGaP diamantane structure using PBEPBE/3-21G

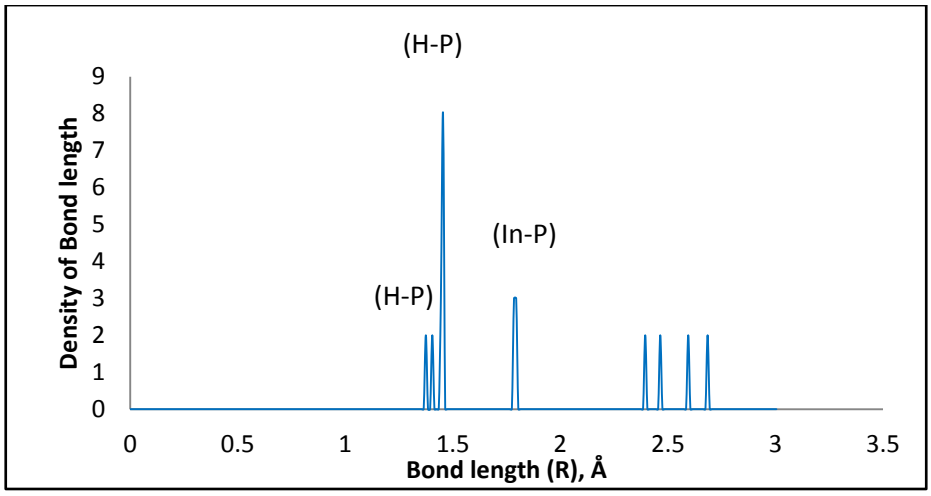


Figure (4). Distribution of Bond lengths (R) in InGaP diamantane with 5 Fluorouracil drug

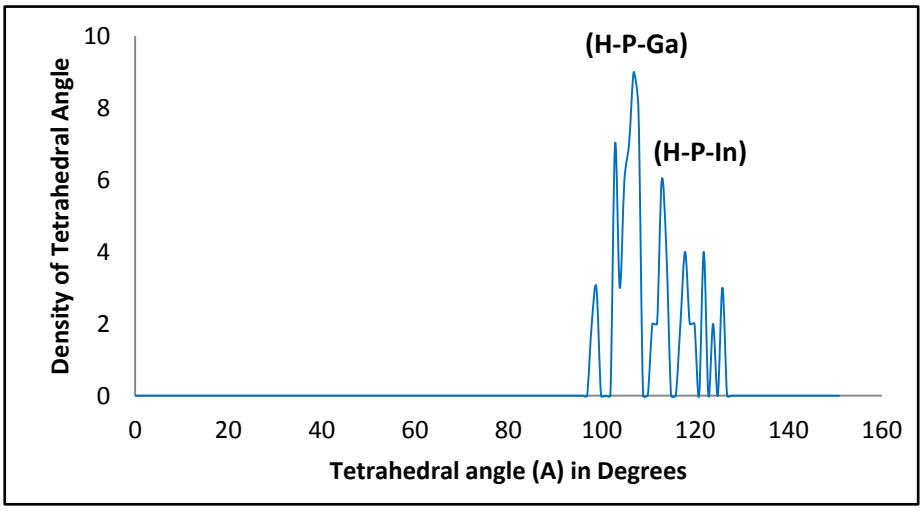


Figure (5). Distribution of tetrahedral angle (A) in degree in InGaP diamantane structure

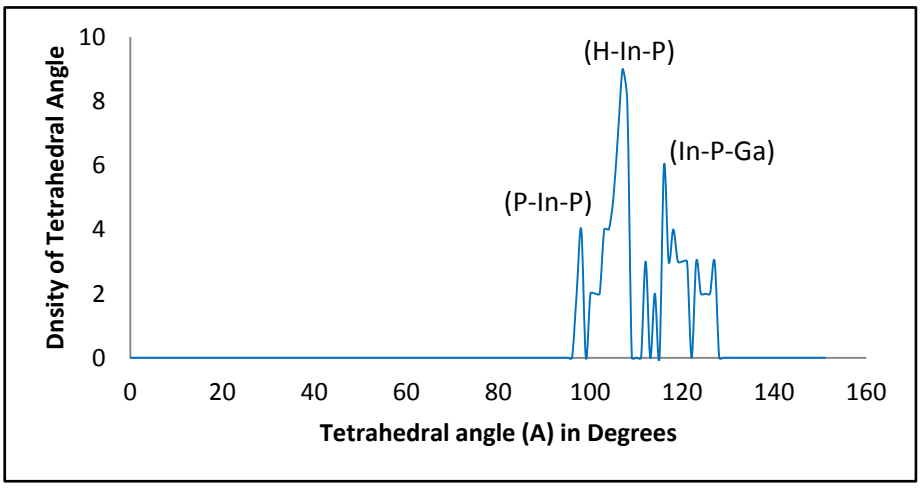


Figure (6). Influence of tetrahedral angle on Density of tetrahedral angle of 5-Fluorouracil-InGaP diamantane

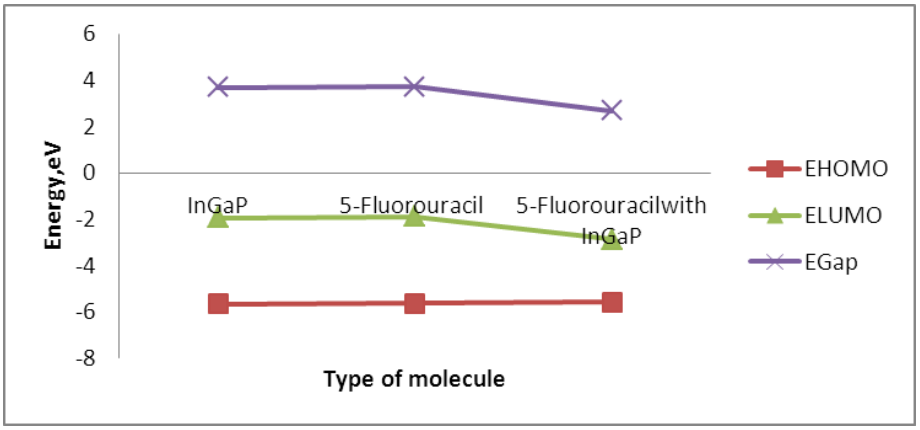


Figure (7). Effect of InGaP binding on the original 5-fluorouracil molecule with different electronic parameters

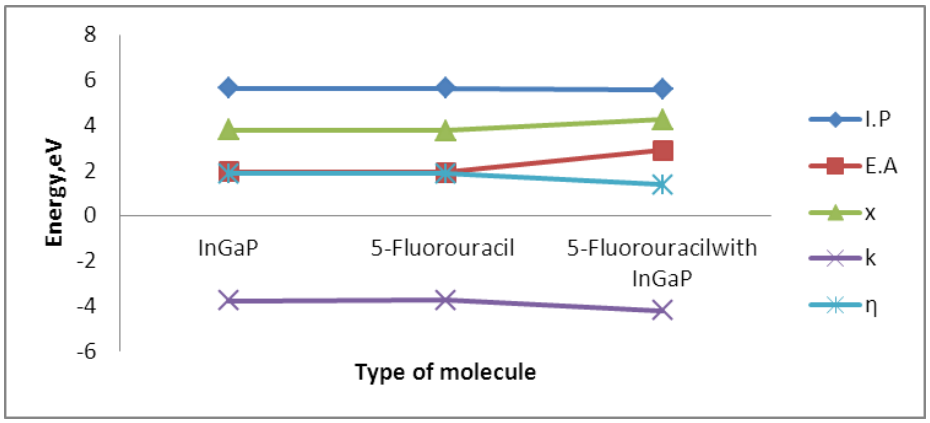


Figure (8). Effect of InGaP binding on the original 5-Fluorouracil with different electronic parameter

It can be seen from Figure (3) that the most thick bond length lays at around 1.44 Å for (H-P) bond and alternate densities are at 1.78 Å for (H-In) bond, 2.62 Å for (H-G) bond. It can be seen from Figure (4) that the most thick bond length lays at around 1.44 Å for (H-P) bond and alternate densities are at 1.79 Å for (In-H) bond, 2.29 Å for (P-Ga) bond as that from Figure (3). Figure (5) can be seen $In_5Ga_2P_7$ tetrahedral angle as (105.831) Å and $In_5Ga_2P_7$ diamantane bonded with 5-Fluorouracil (107.036) Å (Figure 6). Electronegativity, hardness, softness index for InGaP diamantane nanocrystal, 5-Fluorouracil, and with InGaP nanocrystal using PBEPBE/3-21G energy-vertical method, are shown in Figures (7) and (8). The properties that are displayed in Figures (7) and (8) for each property is computed by employing the difference between the total energies of the neutral InGaP diamantane and the ions of InGaP diamantane.

4. Conclusions

The geometry optimization using DFT with either exchange-correlation functional methods (PBEPBE/3-21G) for InGaP diamantane nanocrystal and 5furacil drug has been found in good and suitable to get the electronic properties. This study supplies a new data for 5Fluorouracil – InGaP diamantane nanocrystal for geometry optimization, total energy, and electronic states due to no previous studies for such type of nanocrystal structures.

The total energies for 5Fluorouracil InGaP – diamantane nanocrystal causes decreasing in energy and more stable structure. The result indicates that the InGaP – diamantane working on the transfer drug without interacting with it. This means that the InGaP – diamantane is insulating material and this helps us in the binding process with the drug without the chemical reaction with any medication side effect.

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