MINAR International Journal of Applied Sciences and Technology

Article type : **Research Article**

Date Received : **27/03/2021**
Date Accepted : **15 /04/2021**
Date published : **01/06/2021**

: **www.minarjournal.com**

http://dx.doi.org/10.47832/2717-8234.2-3.3

DENSITY FUNCTIONAL THEORY INVESTIGATION FOR INSB NANOCRYSTAL DIAMANTANE DRUG CARRIER

Methaq Talib MATROOD[1] & Aqeel Adil HASAN[2]

Abstract

Nanomedicine remains the medicinalrequest of nanotechnology. Nanodrugvarietiesafter the medicinalrequests of nanoparticles, to nanoelectronic biosensors, thenuniform possible future applications of particle nanotechnology.Nanoparticle of medicationtransporters are optimized aimed atpreoccupation of medicationsfinishedbreathtreatment. Demonstrating and imitation of nanocrystal limits of the theophylline (C7H8N4O2)byindium – antimony (In7Sb7H20 (in diamantane constructionhave been performed by Gaussian 09 program. DFT hasremainedused for InSb nanoparticle, theophyllinemedication. Optimization and frequency on the ground national level,PBEPBE, 3-21G basis sets consumesremainedexamined. The custodiesaimed ataltogetherremainequivalenttoward zero custodies. The geometry optimization by means of both methods (PBE) for InSb diamantane nanoparticles and theophyllinedrug has been originate cutting-edgedecent agreement by experimental dataMolecular detour theory has been used to discovery highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies. Total energy, ionization potential and electron empathy have beenintendedaimed atInSbnanostructure bytheophyllinemedication.

Keywords: Nanomedicin,Modeling, Diamantane, Drug Carrier, Nanocrystal and InSb.

[1] Iraqi ministry of Education, Iraq, Mithaq988@gmail.com, https://orcid.org/0000-0002-1732-2036
[2] Iraqi ministry of Education, Iraq, aqeel1985adel@gmail.com, https://orcid.org/0000-0001-6263-1615

1. Introduction

The term of density factional theory “DFT” means that remains a calculation quantum mechanical demonstratingtechniquefor physics, chemistry and material knowledgetowardinspect the electronic construction (mainly the ground national) of numerousformschemes, in specificparticles, molecules besidesshortened phase [1]. These biopharmaceuticals current challenges to medication delivery expertsdue to their single nature and trouble in carriagefinishedconservativeways [2]. Theophylline is a methyl xanthine drug used in therapy for respiratory diseases such as asthma [3].Theophylline title includes flat respiratory muscle relaxation, increased air pressure, chronic obstructive pulmonary disease (COPD), and then asthma.[4]. It is not known in what way theophylline reasonsBroncho dilatation in asthmatics. Theophylline constrains phosphodiesterase enzyme and upsurgescellular (cAMP) level [5].The attentiveness of theophylline that constrainsgreatestphosphodiesterase is advanced than the healingvariety, but there is nearly evidence that a subtype of the enzyme (maybekind 4 isoform) in airlineflat muscle is additionalsubtle to the medication. If the sizes of nanoparticleremainlesser than double the Bohr radius for the substantial it is complete of, then quantum imprisonmenthappens [6]. Aimed at the action of humanoidillnesses, adenoidal and pulmonicways of drug delivery are fastcumulative importance [7]. The target of this work is demonstrating and imitation to the formation and project of nanocrystal material of indium antimony, which can be compounded for drug carrier to the place of destination in the humanoid body using diamantane structure.

2- Materials and Methods

Geometry optimization is term for the process thatwork tofind the state of least energy of particle [8]. The processcalculates the wave function then the energy oninitial geometry also proceeds to huntaninitial geometry of a lesser energy [9]. Thatremains repeatpending the lowermostvigor geometry is originate the progressioncomputes the power on apieceparticlethroughassessing the incline (first derivative) of the energy byadmiration to atomic locationsurbane algorithms are then use at apiece step to select a novel geometry [10]. Diamondoids have been of countless attention in new years because of their part in nanotechnology, drug-delivery and medication. The carbon-carbon outline of diamondoids founds the fundamental repeating component in the diamond lattice structure. It remains demonstrate that diamondoids remainactual stable complex [11, 12].

The lesser diamondoid particlesgeneral chemical formulation “C4n+6H4n+12: adamantine (C10H16),diamantane (C14H20), and tiramantane (C18H24)”. Apiece of these three inferior adamantologues consumesonly one isomer [13].Byaprinciple, the possessions of a numerous electron scheme can be strongminded bymeans ofuseful, so thatpurposes of additionalpurpose that in this circumstancestays the spatially reliant on electron thickness [14,15]. Henceforth, the designation“density functional theoryoriginatesafter the usage of useful of the electron thickness [16]. Nanocrystalline semiconductor Indium antimonide (InSb) has been intensively investigated in novel years, because they have many applications in optoelectronics devices counting diodes, transistors, solid-state lasers, and photovoltaic cells [17, 18]. The performance of these devices usually depends on the electronic and optical possessions of the materials used [19]. DFT divider the total energy by way of [20, 21]: $\mathrm{E} = \mathrm{E_T} + \mathrm{E_v} + \mathrm{E_J} + \mathrm{E_{XC}}(1)$

anywhere$\mathrm{E_T}$: refer to “Electronic kinetic energy”, $\mathrm{E_v}$:mains the“Electronuclear interaction energy”, $\mathrm{E_J}$: refer to“Electron-electron disgust”, then$\mathrm{E_{XC}}$: “Exchange correlation period”. Renderingtoward“Koopman's theorm”wherein the edgedetourdynamisms are remained by way of [23]:

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

$\mathrm{E_{LUMO}} = -\mathrm{E.A}(3)$ $I.P$Means thationization potential t then$E.A$refers to the electron affinity.

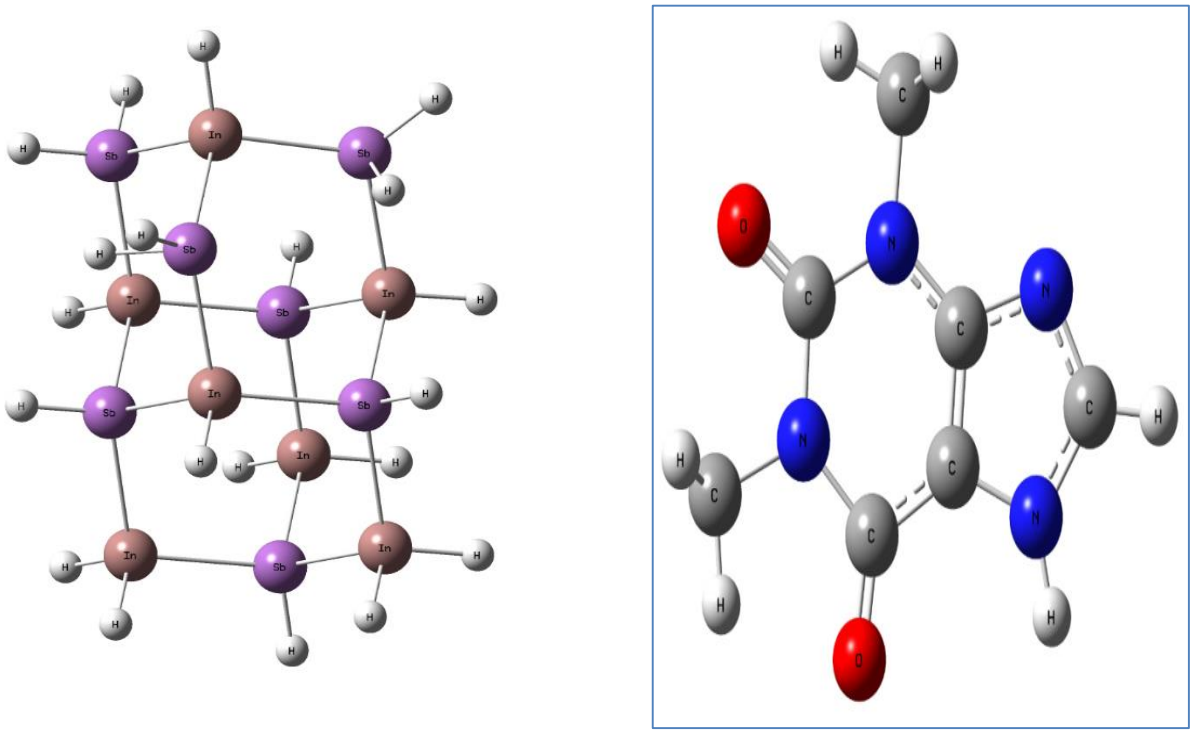
Aimed at the symmetryscheme (e.g. particles), leaseE (N) characterize a crushednationalelectricvigorby way of a purpose of anamount of electrons (N). This one is famous the copied of E(N) byadmiration to (N) on a continuousexterior potential, $V(r)$, the chemical potential (κ) or the electronegativity (χ) of the total negativity are [24]

$\kappa \approx - \mathrm{x} = (\mathrm{IP} + \mathrm{EA})/2(4)$

The theoreticmeaning of “chemical hardness” (η) consumesremainedprovidingthrough the DFTby way of the additionalcopiedfor electronic propertiesbyadmiration to the amount of electrons N at the continuousexterior potential (□) [25].

$\eta = (\mathrm{IP} - \mathrm{EA})/2(5)$

The reckoning (5) demonstrations that chemical hardness remains the confrontation of the chemical potential foralteration in the numeral of electrons of the highest occupied and lowermost unoccupied particledetour (HOMO and the LUMOenergies) of the neutral particlealso it is recognizedby means of orbital-vertical [26]



In7Sb7H20Theophylline(C7H8N4O2)

Fig.(1): the building of InSb (In7Sb7H20) nanocrystal thentheophylline drug (C7H8N4O2)by(PBEPBE/3-21 G)technique

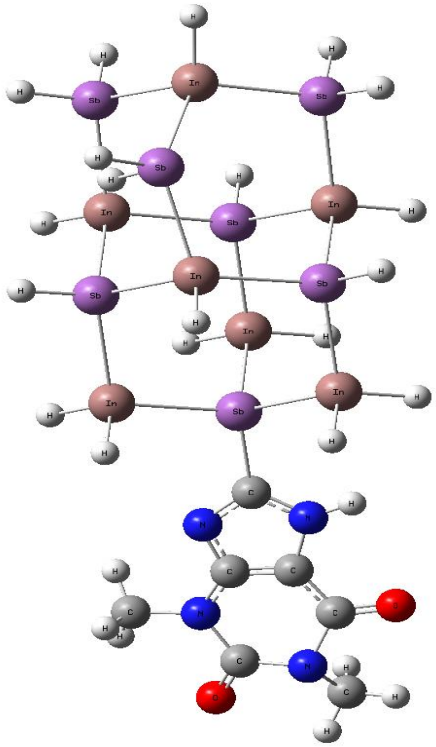


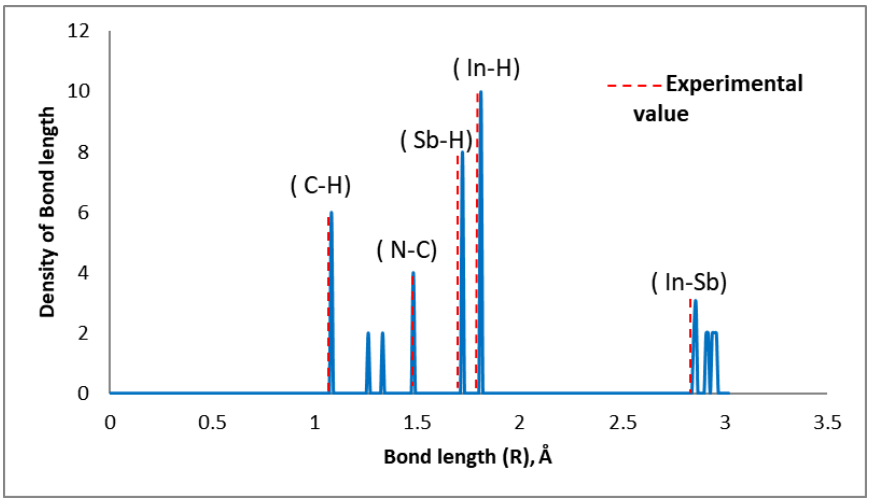
Fig.(2): the building of InSb-theophylline nanocrystal by PBEPBE/3-21 G method

3. **Results and Discussion**

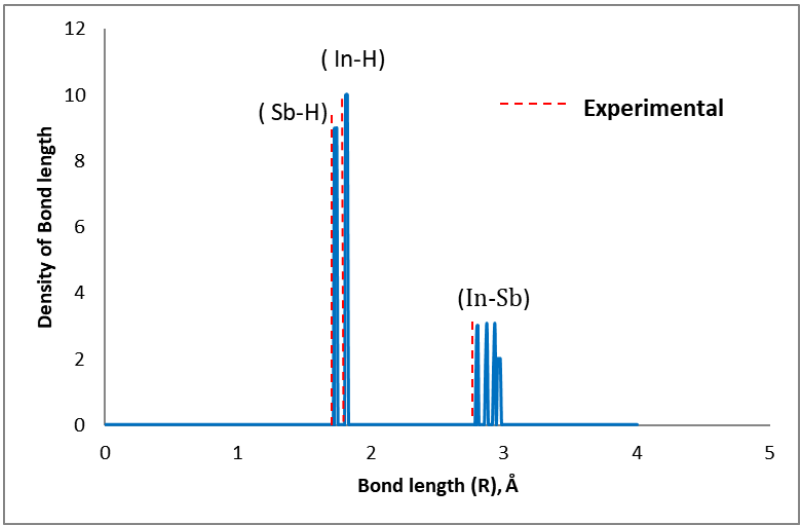
In the present work, used Gaussian program to calculate the optimization limits such as (angles and bonds). Fig.(1) Can be exposed that the geometrical structural of InSb diamantane nanoparticle, Theophylline(C7H8N4O2) then the amount of particles, to these particles in the particle are totaledrenderingtoward their instruction in the particlerequirementunit of the input. Fig. (2) Demonstrations the optimized building of theophylline–InSb Diamantane by PBEPBE/3-21G technique.

Table (1) signifiesa total energy aimed atInSb diamantane, theophylline drug and InSb diamantane compulsory theophylline. The entire energy for InSb diamantane compulsory theophylline is fewer than the total energy for In7Sb7 diamantane.

Table (2)theelectron affinity, ionization potential, Electronegativity and chemical potential willincrease after binding thedrug.

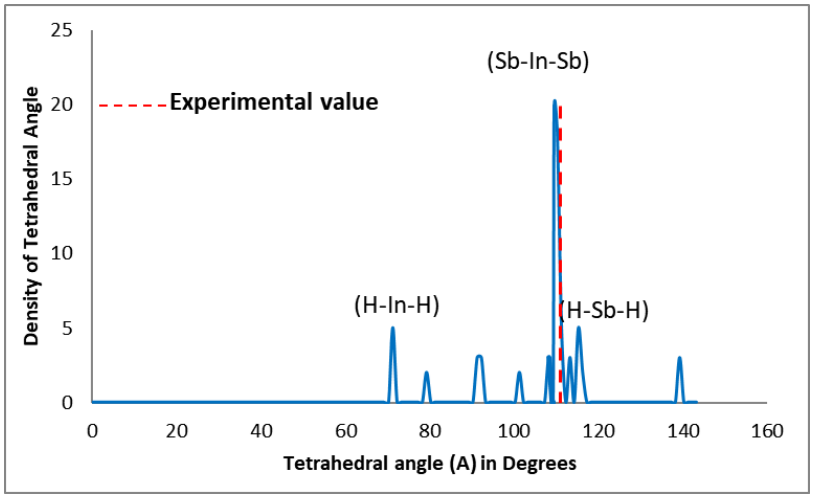


a) Structural parameters of InSbinclude bond length

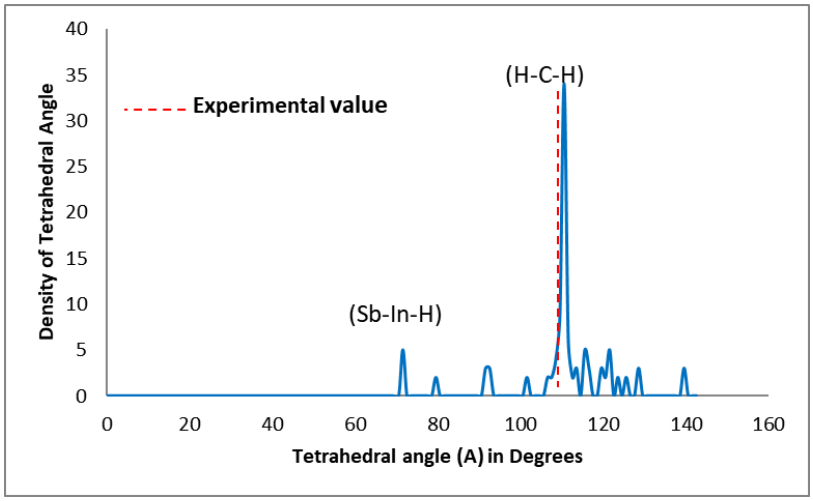


b)Structural parameters of InSb-theophylline include bond length

Figure (3): Structural parameters of InSb and InSb-theophylline include bond length. Experimental value of (bonds length) [13].



a)Structural parameters of InSb that include tetrahedral angles



b) Structural parameters oftheophylline – InSb DiamantaneFigure (4): Structural parameters of InSb and theophylline – InSb Diamantane that include tetrahedral angles, Experimental value. Thecharacteristicworth of tetrahedral angles (109.47 degrees) [11]. Cutting-edge diamond besides ZIncblende constructions.

Table (1). Refer to the Total energy, HOMO, LUMO, and then energy gap aimed at InSb nanocrystal then blinding drug – InSb nanocrystal.

Properties	InSb	Theophylline	InSb with Theophylline
Total energy MeV	-2.287	-0.01733	-2.29759
EHOMO MeV	-4.9583	-5.19104	-5.0209
ELUMO MeV	-4.8149	-1.71619	-4.927
EGap MeV	0.1434	3.4748	0.0939

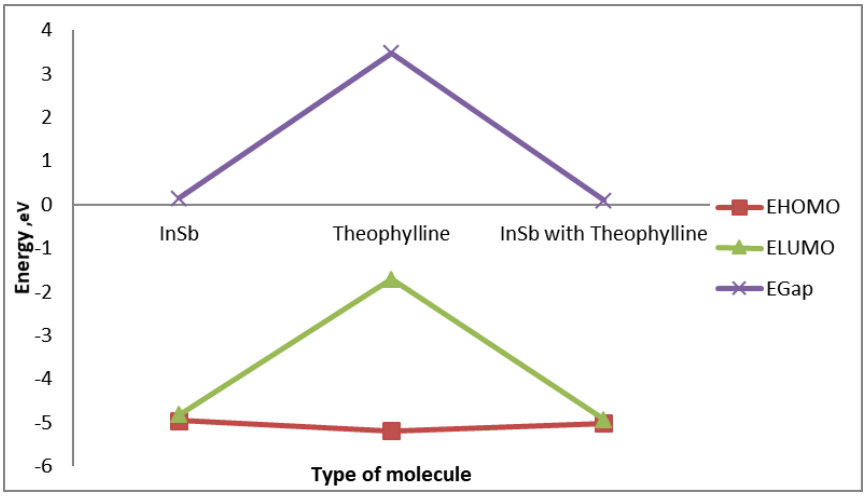


Figure (5). Effect of InSb nanocrystal compulsory on the uniquedrug – InSb, moleculebydissimilar electronic parameters

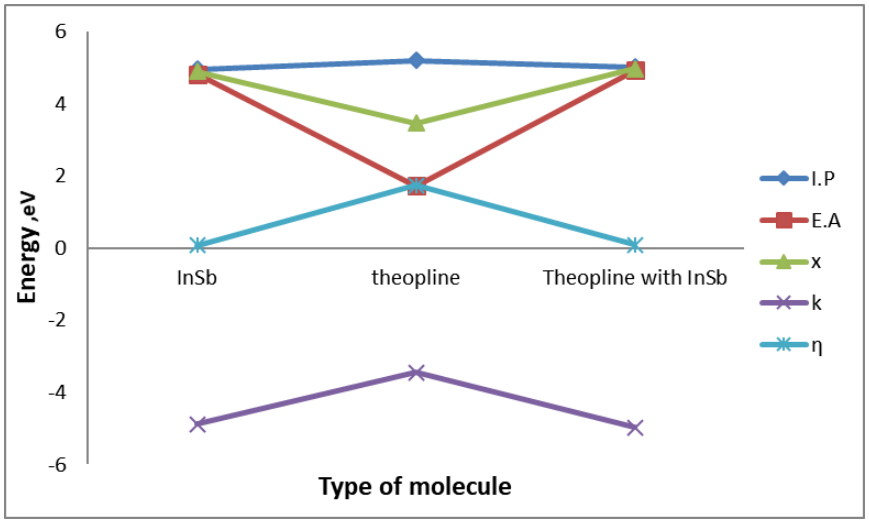


Figure (6). Result of InSb nanocrystal binding on the uniquedrug – InSb, molecule with different electronic parameters

Table (2). Theelectron affinity,ionization potential,Electronegativity, chemical potential,chemical hardnessfor InSb nanocrystal and drug – InSb nanocrystal.

Properties	InSb	theophylline	Theophylline with InSb
E.A	4.8149	1.71619	4.92709
I.P	4.9583	5.19104	5.0209
x	4.8866	3.453618	4.97399
k	-4.8866	-3.45362	-4.97399
η	0.0717	1.7374	0.0939

4. Conclusions

In this work, we can calculation the analytical optimization by means of DFT with also exchange-associationusefulapproaches (PBEPBE/3-21G) aimed at InGaP diamantane nanocrystal and theophylline medicationit wasfound in decent and appropriate to become the electronic possessions. So that the study provisions a novel data aimed attheophylline– InSb diamantane nanoparticle aimed atanalytic optimization, totalenergy, then electronic conditionsbecause of no precedingeducationsaimed at such kindfor nanocrystal constructions.

The entire energies aimed attheophylline InSb – diamantane nanocrystal reasonslesseningfashionable energy thenadditionalsteadyconstruction. The result labelsfor the InSb – diamantane working on the transfer medication without interrelatingbright. Theincome that the InGaP – diamantane is cloistering material. These assistanceswefor the compulsoryprocedureby the medicationdeprived of the chemical reaction byslightlymedicinelateralresult.

References

A. H. Raheem and others "Density Functional Theory Calculations of Thiophene - Phenylene Systems and Their Adducts"JOURNAL OF KUFA – PHYSICS Vol.5/ No.2 (2013)

A. M. Ali " Investigations of some antioxidant materials by using density functional and semiempirical theories" PhD. Thesis, University of Basra, College of Science, Department of Physics, (2009).

A. Szabo; Ostlund, N. S. Modern Quantum Chemistry: Introductionto Advanced Electronic Structure Theory; Dover Publications, Inc.: New York, 1989.

B. Conor Jane and others"The effect of theophylline on the respiratory and quadriceps femoris muscles in man "Adelaide Research & Scholarship (1992).

C. Chen "Ternary Alloy Material Prediction Using Genetic Algorithm and Cluster Expansion " Iowa State University 2015.

C. G. McIntosh, M. Yoonand and S. Berber "Diamond fragments as building blocks of functional nanostructures" Physical Review B 70, 045401 (2004).

C.David Nicholson and others "Differential modulation of tissue function and therapeutic potential of selective inhibitors of cyclic nucleotide phosphodiesterase isoenzymes" Science Direct (1991).

F. N. Ajeel, A. M. Khudair and A. A. Mohammed3, "Density Functional Theory investigation of the Physical Properties of Dicyano Pyridazine Molecules", "International Journal of Science and Research", volume. 4, 4 issue, 1 Janary 2015

G. A. Hafedh Jaber "Study of the Effect of Cyano Subgroup on the Electronic Properties of Azulene Molecule: B3lyp-Dft Calculation " European Scientific Journal December 2013.

G. Onida, L. Reining, A. Rubio - "Electronic excitations: density-functional versus many-bodyGreen's-function approaches " Reviews of modern physics (2002)

H. Ramezani, M. Reza Saberi and G. Ali Mansoori "Diamondoids and DNA Nanotechnologies" (2007).

I. Bâldea "A quantum chemical study from a molecular transport perspective: ionization and electron attachment energies for species often used to fabricate single-molecule junctions" faraday discussions (2014)

J. K. Patra and others "Nano based drug delivery systems: recent developments and future prospects" Journal of Nano biotechnology(2018)

J. Peter Barnes "Theophylline" Pharmaceuticals (Basel)2010.

J. Zevallos and A. Toro-Labbé "A Theoretical Analysis of the Kohn-Sham and Hartree-Fock Orbitals and Their Use in the Determination of Electronic Properties" J. Chil. Chem. Soc. v.48 n.4 Concepción dic. 2003.

K. A. Vivek and G. D. Agrawal "Organic Solar Cells: Principles, Mechanism and Recent Dvelopments" Volume: 03 Issue: 09 | Sep-2014.

K. Capelle "A Bird's-Eye View of Density-Functional Theory" 2006.

L.Raff, R. Komanduri, M. Hagan, S. Bukkapatnam "Neural network in chemical reaction dynamic" Oxford University press (2012).

M. Miller "Phosphodiesterase inhibition in the treatment of autoimmune and inflammatory diseases: current status and potential " Single anonymous peer review 2014.

M.L. Man and others "Theoretical and Computational Chemistry," Acta Phys Chim Sin, vol. 28, pp. 51-57, 2012.

N. S. Babu “Computational Studies and Multivariate Analysis of Global and Local Reactivity Descriptors of Five Membered Heterocycles Molecules by Density Functional Theory (DFT)" International Journal of Pure and Applied Researches; Volume 1(1)/2015.

P.J.Hassnip, K. Refson and Others "Density functional theory in the solid state”Philos Trans a Math Phys Eng Sci 2014.

S.D. Sholl and j. a. steckel "Density functional theory: a practical introduction" Wiley (2009).

T. Kasim and A. Al-Raheem "Ab-Initio Study the Electronic Structure of InXGa1- XP Nanocrystals" (2013).

T. Kasimand M. T. Hussein "Study of the Electronic Structure of Indium Gallium Phosphide In0.5Ga0.5P Nanocrystals "Iraqi Journal of Physics, 2012.

Y. A. Al Shaabania, B.B. Kadhim, F. H. Jasim"Structural and Electronic Properties of Theophylline-InPDiamantane Drug Carrier " , American Scientific Research Journal for Engineering, Technology, and Sciences (2016)