Density Functional Theory Calculations of Electronic Properties ,IR and UV-Vis Spectrum , Dipoles Moments ,and Atomic Charge Distribution of Mg $_{1-X}$ Zn $_XFe_2O_4$ Ferrite

Hashim Ali Yusr

Dept. of Physics-College of Science-Wasit University

hashim@uowasit.edu.iq

المستخلص

أستخدمت طريقة نظرية دالة الكثافة DFT واستخدام الدالة B3LYP و مجموعة اساس basis set المراسة فيرايت السبنل مغنسيوم-زنك ذات الصيغة الكيميائية Mg_{1-x}Zn_xFe₂O₄ .أستخدمت طريقة DFT لاجراء حسابات للتركيب المثالي و الحالات الالكترونية (HOMO-LUMO) و الخصائص الالكترونية مثل (جهد التاين و الكهروسالية والألفة الالكترونية ,والالكتروفلك و الصلادة الكيميائية والنعومة التي تمثل قابلية التفاعل) و. تم اجراء حسابات نظرية لرسم طيف الموجات تحت الحمراء وطيف الموجات فوق البنفسجية لهذه الجزيئات. تم حساب جميع انواع العزوم الكهربائية للفيرايت وكذلك توزيع Mullikan و NBO لفيرايت السبنل Mg_{1-x}Zn_xFe₂O₄ . و الخصائص تم حساب جميع منه الموجات تحت الحمراء وطيف الموجات فوق البنفسجية لهذه الجزيئات. تم حساب جميع انواع العزوم الكهربائية للفيرايت وكذلك توزيع Mullikan و NBO فيرايت السبنل Gauss view 5.08 مع برنامج Gauss view 5.08 مع برنامج Gauss view 5.08 مع برنامج Gauss view 5.08 مع التي الخرام (d,p)

Abstract

Theoretical study using (Density Functional Theory) DFT method with B3LYP functional and the 3-21G(d,p) basis set had been implemented of calculating molecular structure properties of Magnesium – Zinc spinel ferrite having the chemical formula $(Mg_{1-x}Zn_xFe_2O_4)$. DFT had been used to optimize molecular structure, electronic state (HOMO-LUMO), and electronic properties (ionization potential, electronegativity, electron affinity, electrophilic, hardness, and softness) are calculated. Theoretical electronic IR spectrum were computed and plotted . UV-Vis spectrum calculated and plotted of this molecule. Dipole, Quadrupole, and Traceless Quadrupole moments were calculated. The Mullikan and Natural Bond Orbital (NBO) distribution of $Mg_{1-x}Zn_xFe_2O_4$ compound are also computed by DFT. All these properties had been calculated using Gaussian09 program with Gauss view 5.08 program by using (Density Functional Theory) DFT method with 3-21G(d,p) basis set.

Keywords: DFT Calculations, Electronic Properties, IR Spectra, UV-Vis Spectrum, Atomic Charge Distributions, Ferrite

Introduction

ferrites are a type of ceramic compound and sintered material and they are with magnetic properties used in many types of electronics devices[1] . Ferrites are composed of iron oxides with other metals in chemical combination. they known as(ferrimagnetic materials) and (ferrites), and they are electrically nonconductive material therefore ferrites are electrical insulation and mainly used in high frequency devices[2][3] .the important properties of ferrites are hard, brittle, polycrystalline, iron containing, and gray or black. Electrical resistivity for ferrites is so high therefore eddy current losses is very low at high frequencies .There are three types of ferrites due to their structure : spinel, hexagonal, and garnets are ferrites, and there are two types of ferrites due to their (magnetic coercivity), soft ferrites have low coercivity and hard ferrites have high coercivity. Figure (1) shows soft and hard ferrites and their hysteresis loops[4][5].



Small loop area = low hysteresis loss Large loop area = high hysteresis loss

Fig.(1) Hysteresis loop for (a) soft ferrites and (b) hard ferrites [6]

Manganese-Zinc Ferrite

Manganese-Zinc Ferrite is a cubic spinel ferrite. The general formula for spinel AB_2O_4 where A and B ferrites are represent cation sites for tetrahedral and octahedral respectively Fig.(2), and also the formula may be written as MeO Fe_2O_4 where Me is a divalent metal cation for example Mn, Co, and Zn and the formula of Mn-Zn feriite is($Mg_{1-x}Zn_xFe_2O_4$) [7][8] . The structure of spinel ferrites like the structure of the mineral spinel MgAl₂O₄, and ther are different distribution of cations : normal ,mixed, and inversed spinel ferrites. Mn-Zn high has permeability in RF region, high resistivity ,mechanical hardness ,and chemical stability. The sintering temperature about 1350 ⁰C for Manganese-Zinc Ferrite to attain the preferred manipulate on

octahedral and tetrahedral sites for the Mg^{2+} ions distribution [9][10][11].



Fig.(2) The unit cell structure for spinel ferrite [6]

Density Functional Theory (DFT)

Density functional theory DFT is a ground state theory and one of the essential and successful quantum mechanical methods in physics and chemistry, and has lengthy been the best method of electronic structure calculations in solid stat physics fields. DFT had been used to calculate electronic structure basically the ground state of (many body systems), specifically atoms. and molecules .The characterization of a many electron systems can be determined via the usage of functional, (functions of another function), which in this situation is the spatially established electron density. The name density functional theory refer to using functional of the electron density. Methods of electronic structure had been used to find approximate solutions of Schrodinger equation of N-interacting

electrons which are move in an, external and electrostatic potential. DFT is the famous and flexible methods in computational physics ,and since the 1970s it is very popular in solid-state physics calculations.

There are many approximations were used in DFT and computational costs were became so low comparison with other traditional methods. [12][13][14]

Overview of DFT

The Schrödinger Equation

Schrodinger equation gives important informations for many phenomena in complex systems. Wavefunction defines stationary electronic state and used to satisfy time -independent Schrodinger equation for *N*-particles interacting [15]:

$$\hat{\mathbf{H}}\Psi = E\Psi \tag{1}$$

H : Hamiltonian operator which describes both the kinetic and potential energies of electrons and nuclei.

E : the energy of an electron which it is at a (distance r) from a nucleus of Z-charge.

 Ψ : The wavefunction depends on the electron coordinates .

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For Many electrons (atoms/molecules) [16]:

$$\hat{\mathbf{H}} = \sum_{i}^{electrons} \frac{-\hbar^{2}}{2m_{e}} \nabla_{i}^{2} + \sum_{A}^{nuclei} \frac{-\hbar^{2}}{2m_{A}} \nabla_{A}^{2} + \sum_{i}^{electrons} \sum_{A}^{nuclei} \frac{-e^{2}Z_{A}}{r_{iA}} + \sum_{i>j}^{electrons} \frac{e^{2}}{r_{ij}} + \sum_{A>B}^{nuclei} \frac{e^{2}Z_{A}Z_{B}}{r_{AB}}$$

$$(2)$$

where

 $\sum_{i}^{electrons} \frac{-h^2}{2m_e} \nabla_i^2$ is the kinetic energy of the

electrons

 $\sum_{A}^{nuclei} \frac{-h^2}{2m_A} \nabla_A^2$ is the kinetic energy of the

nuclei

 $\sum_{i}^{electrons} \sum_{A}^{nuclei} \frac{-e^{2}Z_{A}}{r_{iA}}$ is the electrostatic

interaction between the electrons and the nuclei

$$\sum_{i>j}^{electrons} \frac{e^2}{r_{ij}}$$
 is the electrostatic interaction

between the electrons

 $\sum_{A>B}^{nuclei} \frac{e^2 Z_A Z_B}{r_{AB}}$ is the electrostatic-interaction

for the nuclei.

The solution of the Schrodinger equation with H_{elec} is the electronic wavefunction Ψ_{elec} and the electronic energy E_{elec} . The total energy E_{tot} is then the sum of E_{elec} and the constant nuclear repulsion term E_{nuc} .

Born-Oppenheimer Approximation

If the nuclei are constant and do not moveing, therefore their kinetic energy must be zero. Potential energy is constant because it depend on repulsion of nucleus-nucleus. The Hamiltonian in equation (2) reduces to the so-known electronic Hamiltonian [17][18]:

$$\hat{\mathbf{H}}_{el} = \sum_{i}^{electrons} \frac{-\mathbf{h}^{2}}{2m_{e}} \nabla_{i}^{2} + \sum_{i}^{electrons} \sum_{A}^{melei} \frac{-e^{2}Z_{A}}{r_{iA}} + \sum_{i>j}^{electrons} \frac{e^{2}}{r_{ij}} + \sum_{A>B}^{melei} \frac{e^{2}Z_{A}Z_{B}}{r_{AB}}$$
(3)

The solution of Schrodinger equation for $\hat{\mathbf{H}}_{el}$ is the (electronic wavefunction) Ψ_{el} , and the (electronic energy) E_{el} . The (total energy) E_{tot} is sum of E_{el} and the constant (term of nuclear repulsion) E_{nuc} :

$$\hat{\mathbf{H}}_{el} \Psi_{el} = E \Psi_{el} \qquad (4)$$
$$\mathbf{E}_{tot} = \mathbf{E}_{elec} + \mathbf{E}_{nuc} \qquad (5)$$

• Variational Theorem

If a system in Ψ_0 state, then (expectation value of energy) [18] [19]:

$$"E = \frac{\int \Psi_{el}^* \hat{\mathbf{H}}_{el} \Psi_{el} d\tau}{\int \Psi_{el}^* \Psi_{el} d\tau} "$$
(6)

The variational principle states that " the energy of any guess wavefunction must be larger than or equal to the true energy calculated with the accurate wave function; the closer the guess to the true wave function, the lower the energy based on the guess wave function. The guess wave function that produces the lowest energy is thus the best approximation to the true wave function"[20].In other words, the ground state energy is a functional of the number of electrons N and the nuclear potential $V_{ext"}$ [18] [19]:

$$E_{o} = E[N; V_{ext}]$$
(7)

• The Hartree-Fock Approximation

If the ground state wavefunction Ψ_{0} is an antisymmetrized product of N-orthonormal spin orbitals Ψ i(x), for N electrons the Slater determinant[21][22] :

$$\Psi(\mathbf{x}_{1},\mathbf{x}_{2},\mathsf{K},\mathbf{x}_{N}) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \chi_{i}(\mathbf{x}_{1}) & \chi_{j}(\mathbf{x}_{1}) & \dots & \chi_{k}(\mathbf{x}_{1}) \\ \chi_{i}(\mathbf{x}_{2}) & \chi_{j}(\mathbf{x}_{2}) & \dots & \chi_{k}(\mathbf{x}_{2}) \\ \vdots & \vdots & \ddots & \vdots \\ \chi_{i}(\mathbf{x}_{N}) & \chi_{j}(\mathbf{x}_{N}) & \dots & \chi_{k}(\mathbf{x}_{N}) \end{vmatrix}$$
(8)

Where rows represent electrons, and columns correspond to orbitals. In Hartree-Fock approximation the orthogonal orbitals Ψ_i are found the energy is minimize for this determinantal form of Ψ_o :

$$"E_{\rm HF} = \min(\Psi_{\rm HF} \rightarrow_{\rm N})E[\Psi_{\rm HF}]" \qquad (9)$$

• The Electron Density

The electron density is the important quantity in DFT. It's definition is the integral over the coordinates of spin of all electrons and over all but one of the (spatial variables) ($\mathbf{x} \equiv \mathbf{r}$,s) $x_1, x_2, \dots x_N$

$$\rho(\mathbf{r}) = \mathbf{N} \int \dots \int |\psi(x_1, x_2, \dots, x_N)|^{-2} dx_1 dx_2 \dots dx_N \quad (10)$$

where $\rho(\mathbf{r})$ calculate the probability of any of N-electrons within volume element d \mathbf{r} .

• Thomas-Fermi model

the kinetic energy based on (uniform electron gas) was proposed in 1927 and it is consider as a first density functional theory [23]:

$$[\rho(\mathbf{r})] = \frac{3}{10} (3\pi^2)^{2/3} \int \rho^{5/3}(\mathbf{r}) d\mathbf{r} \operatorname{T}_{\mathrm{TF}^{(11)}}$$

the (nuclear-nuclear) potential and the (electron-electron) potential for the classical expression represent the atom's energy [23]:

$$T_{\rm TF} \left[\rho(\boldsymbol{r}) \right] = \frac{3}{10} \left(3\pi^2 \right)^{2/3} \int \rho^{5/3} (r) dr - \int \frac{\rho(r)}{r} d\frac{1}{2} \iint \frac{\rho(r1)\rho(r2)}{r12} dr 1 dr 2 \qquad (12)$$

The energy is given absolutely in terms of electron density.

• The Hohenberg-Kohn Theorems.

The Hohenberg-Kohn theorems had been related to a system that consist of electrons have been moved under the influence of an (external potential).First theorem state that [24]" the external potential $V_{ext}(r)$ is determined (within a trivial additive constant) by the electron density $\rho(r)$ "Second theorem state that[24]" the functional $F_{HK}[\rho]$ that

delivers the ground state energy if and only if the input density is the true ground state density"The two theorems are give the essential statement of (density functional theory) DFT.

Computational Details

Density Functional Theory methods has been performed by using the Gaussian 09 and Gauss view 5.08 program9 [25]. the geometric optimization of ZnMgFe₂O₄ molecules have been performed with B3LYP/3-21G(d,p) basis set .B3LYP has been used to calculate the electronic properties for molecule such as (electronic energy gaps, and ionization states, potentials). HOMO, The highest occupied molecular orbital and the LUMO, the lowest Unoccupied Molecular Orbital have been used to calculate electronic potential (IP) and electron affinities (EA) [26] [27]:

$$IP = -E_{HOMO}$$
(13)

$$EA = - E_{LUMO}$$
(14)

The chemical potential (μ) , defined as" a measures of the escaping tendency of an electronic cloud, and this factor equals the slope of the Energy versus N (number of electrons) at external potential v(r) "[28][29]:

$$\mu = \left[\frac{\partial E}{\partial N}\right]_{\nu(r)} \tag{15}$$

The electronegavity χ was calculated as [27] [28] :

$$\mu \approx -\chi = -(IP + EA)/2 \tag{16}$$

The hardness defined as "the second derivative of electronic energy with respect to the number of electrons N, for a constant external potential v(r)" [27] [28] :

$$\eta = \frac{1}{2} \left[\frac{\partial^2 E}{\partial N^2} \right]_{\nu(r)} = \frac{1}{2} \left[\frac{\partial \mu}{\partial N} \right]_{\nu(r)}$$
(17)

The hardness has been calculated as [30][31]:

$$\eta = (IP - EA)/2 \tag{18}$$

that mean hardness equal half of the energy gap $(E_{HOMO} - E_{LUMO})$.

the softness is has been calculated as [31][32]:

$$S = \frac{1}{2\eta} = \left(\frac{\partial^2 N}{\partial E^2}\right)_{\nu(r)} = \left(\frac{\partial N}{\partial \mu}\right)_{\nu(r)}$$
(19)

Electrophilic index defined" as a measure of energy lowering due to maximal electron flow between donor and acceptor". Electrophilic index ω given as[31] [32]:

$$\omega = \frac{\mu^2}{2\eta} \tag{20}$$

The electric dipole polarizability is define as "a measure of the linear response of the electron density F,and represents a second-order variation in the energy"[33][34]

$$\alpha = -\left(\frac{\partial^2 E}{\partial F_a \partial F_b}\right)_{a, b} = x, y, z$$
(21)

Polarizability $\langle \alpha \rangle$ was given by the equation [33][34]:

$$<\alpha>=\frac{1}{3}(\alpha_{xx}+\alpha_{yy}+\alpha_{zz})$$
 (22)

Where

 $\alpha_{xx} \leq \alpha_{yy} \leq \alpha_{zz}$: eigenvalues of the polarizability tensor.

Result and Discussion

Molecular Geometry

Figure (3) shows the geometric optimization of $ZnMgFe_2O_4$ molecules by using DFT method. Figures (4) and figures (5) had been showed E_{HOMO} and E_{LUMO} .



Figure (3) the geometric optimization of ZnMgFe₂O₄ molecules



Figure (4) HOMO the energy of the highest occupied molecular



Figure (5) LUMO the energy of the lowest unoccupied molecular orbital.

Electronic Properties

Table (1) shows the calculated values of HOMO and LUMO and energy gap between them, and electronic properties IP, EA , χ , η , S and w. all properties are computed by using DFT/B3LYP 3-21G(d,p) method .

Table(1)HOMO,LUMO,andElectronic properties (IP,EA,χ, η, S, andW) measured in eV units

E _{HOMO}	-5.64421
E _{LUMO}	-2.5243
Eg	3.119913
IP	5.644213
EA	2.5243
χ	4.084257
η	1.559957
S	0.320522
W	5.346672

IR spectra

Figure (6)has been showed The IR spectra .Harmonic vibrational frequencies are computed using B3LYP level using the 3-21G(d,p) basis set.



Figure (6) IR spectra

peaks in fig.(6) are due to the spinel structure and is attributed to the intrinsic vibrations of octahedral coordinated metal ions in the spinel structure. Infrared spectra has been occurred when the absorb frequencies for molecules are characteristic of molecular structure. All these absorption has been occurred at resonant frequencies. That's mean the absorbed radiation frequency matches vibrational frequencies.

The UV-Visible spectrum

Figure (7) shows UV-Visible spectrum the spectra computed by an excited states calculation. UV-Vis spectrum is correspond to the excitation of a molecule from the electronic ground state to electronically excited states with simultaneous excitations of vibrational, rotational . The DFT/B3LYP method using basis set 3-21G which used to determine the first three low-lying excited states for investigate the UV-V is absorption spectra of the title compound at TD-DFT(C-PCM)/ 3-21G. The calculated results wavelength are performed .



Fig. (7) The UV-Visible spectrum

Dipoles moments

Dipoles moments in all types such as Dipole, Quadrupole, Quadrupole, Traceless Quadrupole moments this shown in table (2) The dipole moment is in addition an important physical property. Dipole moments have been occured when there is a separation of charge. They can occur between two ions in an ionic bond or between atoms in a covalent bond; electronegativity has been asised by dipole moments . The larger the difference in electronegativity, the larger the dipole moment. the size of the dipole moment is affected by the distance between the charge separation ,and The dipole moment is a measure of the polarity of the molecule.

Dipole moment (field independent basis, Debye):					
X= 4.0793	Y=3.47		Z=2.923		Tot -6 1065
		91	2		101 -0.1005
Quadrupole moment (field independent basis, Debye Ang):					
XX= 83.3492	YY= 83		.1071 ZZ= 6		ZZ= 65.1417
XY= 1.9102		YZ= 2.	6506		XZ= 1.6525
Traceless Quadrupole moment					
(field independent basis, Debye Ang):					
XX= 6.1499		YY=	5.9078		ZZ=12.0576

Table(2) dipole moments of ZnMgFe₂O₄

Atomic Charge Distributions

A (Natural Bond Orbital) NBO has been calculated bond orbital together with maximum electron density.

The Mullikan and Natural Bond Orbital (NBO) distribution of ZnMgFe2O4 compound are computed on B3LYP method using 3-21G basis set. The calculated values of the charges are listed in Table (3).The charge distribution of the title compound shows that the iron 'Fe",

Zinc"Zn" and Magnesium "Mg "atoms are positive charges due to the presence of electronegative Oxygen" Table(3)TheMullikanchargesofZnMgFe2O4calculatedbytheB3LYPmethodwith 3-21Gbasisset

Atom	Mullikan	(NBO)
	Atomic	Charges
	Charges	
1 Fe	0.517911	0.295470
2 O	-0.198584	-0.078252
3 O	-0.381857	-0.115433
4 O	-0.459444	-0.157870
5 O	-0.414641	-0.269697
6 Fe	0.282938	0.159775
7 Mg	0.378364	0.135628
8 Zn	0.275314	0.030379

Conclusion

1.The Density Functional Theory (DFT) method with B3LYP/3-21G level has been found a good results in calculation geometrical parameters, fundamental vibrational frequencies and exciting energies in comparison with experimental data.

- 2. The HOMO (an electron donor) and LUMO (an electron acceptor) defferent energies gave values of energy gaps of ZnMgFe₂O₄ the theoretical calculation using Gaussian 09 programs obtained E_g (3.119 eV).
- 3. The UV-VIS and IR spectrum using DFT methods have a good agreements with experimental results.

4. Atomic charge distribution show that the increasing distance, compound with ferrites group showed the higher dipole moment.

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