Sudan University of Science and Technology
College of Graduate Studies

Electronic Band Structural Calculation of $CeCrO_3$Perovskite Compound as Paramagnetic and ferromagnetic: Density Functional Theory (DFT) Study

حساب هيكلية النطاق الالكتروني لمركب البيروفسكايت $CeCrO_3$عن طريق نظرية الكثافة الوظيفية كاحادية وحديدية المغناطيسية

A thesis Submitted in Partial Fulfillment for the Requirement of a Master Degree (M. Sc) in Physics

By

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I thank Allah who made all these possible.

Abstract

The perovskite compounds is materials most used in solar cell applications. In this thesis, were studied and calculated electronic band structure of perovskite compound CeCrO3 by using quantum espresso software based on density functional theory (DFT), plane wave(PWSCF) and pseudo-potential(P.P) in ground state energy level. And were found the material has very small band gap and were could not used in semiconductor application. To solve that problem were change the direction of spin and after that the properties of material will change from paramagnetic to ferromagnetic and were got high lattice parameter, band gap, density of state than the paramagnetic.

الملخص

مركبات البيروفسكايت هي مواد معظم استحداماتها في تطبيقات الخلايا الشمسية. في هذه الأطروحة دُرست وحُسبت تركيب النطاق الالكتروني لمركب البيروفسكايت $CeCrO_3$ باستخدام برنامج الكوانتم اسبريسو علي اساس نظرية الدالة الوظيفية (DFT) والموجة المستوية (PWSCF) وجهد (Pseudo) في مستوي الطاقة الارضي. واوجدنا ان المادة لديها فجوة نطاق صغيرة ولا يمكن استخدامها في تطبيقات اشباه الموصلات. ولحل هذة المشكلة غُير اتجاه الاسبين وبعد ذلك تغيرت خصائص المادة من احادية المغناطيسية الي حديدية المغناطيسية $CeCrO_3$ وحصلنا علي مقياس الشبيكة وفجوة الطاقة وكثافة الحالة اكبر من المادة احادية المغناطيسية.

Table of contents

Chapter Three

Chapter Four

Chapter Five

References

LIST OF THE FIGURES

List of tables

Abbreviations

DFT	Density functional theory.
PWSCF	Plane wave self consistent field.
P.P	Pseudo-potential.
CMOS	Complementary metal oxide semiconductor.
FCC	Face centered cubic.
BCC	Body centered cubic.
LDA	Local density approximation.
GGA	Generalized gradient approximation.
QE	Quantum espresso.
DOS	Density of states.

Chapter One

Introduction

1.1General Overview:

A perovskite structured compounds consist of inorganic and hybrid organic_ inorganic material and the general formula is ABX_3. The most prominent application of these perovskite is solar cells. This material are cheap to produce and simple to manufacture and the engineering improvements of perovskite formulations and fabrication routines has led to significant increases in power conversion efficiency in a few year about 22.1%. Although the perovskite produce power with high efficiency but it was suffer many problems most commonly stability, sensitive to high temperature , UV_ light , moisture , oxygen and most efficiency absorbers in corporate lead. Therefore, there are great chance for more research into the physics and chemistry around perovskites (Shi & Jayatissa, 2018).

The perovskite compound of $CeCrO_3$ include Cr is a trivalent ion of one of the transition group elements that are used to study magnetic properties of $CeCrO_3$. The natural situation of $CeCrO_3$ from periodic table is paramagnetic material according to properties of Cr , when we change the direction spin of electron of $CeCrO_3$ from paramagnetic to ferromagnetic material, we will get lattice parameter and band gap and density of state high than paramagnetic material.

1.2The Problem Statement

At some stage the experimental approach is expensive and hard to find. The other way to calculated the important properties of some compound can be achieve by using other techniques such as simulation. The natural situation of CeCrO3 from periodic table is paramagnetic material according to properties of Cr. This from of this compound possesses very small band gap, which cannot classify it is as semiconductor. In this dissertation we studied the electronic band structure of CeCrO3 as ferromagnetic and paramagnetic, and the comparison was made.

1.3 General Objectives

- Studied and calculated electronic band structure of CeCrO3 compound.

1.4 Specific Objectives

- Review the DFT method.
- Review perovskite compound of CeCrO3.
- Using quantum espresso software based density functional theory for structural optimization and to calculate electronic band structure and density of state of CeCrO3 as paramagnetic and ferromagnetic.

1.5 layout of the dissertation

This thesis is constructed as the follow: in chapter one we give a concise introduction. The pervious study of perovskite Compound of $CeCrO_3$, Density Functional Theory are reviewed in chapter two. Chapter three touched upon the method and simulation software, how to use data entry, numerical result in chapter four. discussion, conclusion and recommendation are presented in chapter five.

Chapter Two

Theoretical Background

In this chapter, the complete studies of the perovskite compound $CeCrO_3$, density functional theory are presented.

2.1 Pervious Studied

By considering density functional theory (DFT) in terms of investigation, we have explored the structural, electronic and magnetic properties of cubic $CeCrO_3$ for the first time. In order to determine the structural stability of cubic $CeCrO_3$ compound, we optimized the structure of $CeCrO_3$ in non-magnetic (NM), ferromagnetic (FM) phases by using PBE generalized gradient approximation (GGA) functional to find the exchange-correlation potential. From structural optimization, the FM phase of $CeCrO_3$ is observed to be stable.

Perovskite oxides get so much attention due to its effective use in gas separation membranes, solid fuel cell and piezoelectric. Lanthanide doped perovskite type oxides, for example $CeCrO_3$ (Ce: lanthanides, Cr: transition metals), have been accustomed for functional inorganic materials having inclusive diversity of applications for alkaline fuel cells electrodes , gas ions sensors and catalysts for fast and complete oxidation/reduction of CO, NO and other hydrocarbons Various fascinating physical properties such as structural, electronic, optical and magnetic properties are inter-dependent in transition-metal oxides. These materials are predictable for spintronics devices effectively. The association of magnetic and electronic played a role to develop the research in area of spintronics. Half-metallic ferromagnetism has a significant part because of its spin- polarization at the Fermi-level which is necessary for the better performance of spintronic applications. All these points force us to explore half-metallic Ferro-magnets with important magnetic moment that well-matched with existing semiconductor technology. Material similar to half-metal have a unique property to act as conductor in one direction of spin and insulator for opposite direction, therefore, it is very suitable for device applications and get attention for researcher that are working in the area of spintronic devices. Some major example are magnetic disk drives, magnetic tunnel junctions, magnetic hybrid technology for CMOS and magnetic sensor, non-volatile magnetic random access memories.

Several research groups perform numerous experimental and computational studies on the half-metallic Ferro-magnets, and many half-metallic materials have been predicted and experimentally verified. As it can properly find electronic and magnetic characteristics. The structural properties of aforesaid crystals are calculated at ground state and equated with the prevalent theoretical and experimental data (Rashid, Iqbal, & Noor, 2017).

2.2 Definition of perovskite compound $CeCrO_3$

The perovskite structure has the general formula of ABX_3, where A and B are cations and X is an anions. In perovskite mineral $CeCrO_3$ the Ce, Cr are trivalent, Ce of the rare earth elements and Cr of the transition elements. The general shape of perovskite lattice is that it consists of A cation at corner of a cube and B cation within oxygen octahedral, $CeCrO_3$ exhibits face centered cubic lattice structure with space group $Pm^{-}3m$ (Chapter 3 Perovskite Perfect Lattice - Atomistic Simulation ...[PDF], 201).

The band gap of this compound is very small is about 0.011ev from data base if we considered this material as paramagnetic material. This is a major problem because we could not studied optical properties and also could not use as semiconductor for solar cell application.

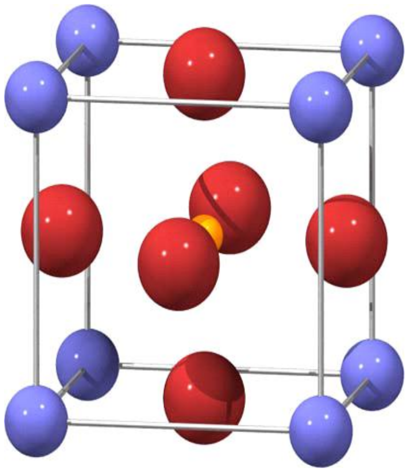


Figure 2.1: Cubic perovskite unit cell. Blue spheres represent the A cations, yellow spheres represent the B cations, and red spheres represent oxygen anions forming an octahedral.

Table (2.1): Atomistic positions in cubic perovskites

Site	Coordinates
A cat ion	(0,0,0)
B cat ion	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
O anion	$(\frac{1}{2},\frac{1}{2},0)$ $(\frac{1}{2},0,\frac{1}{2})$ $(\frac{1}{2},\frac{1}{2},0)$

This atomistic position in the direct lattice with volume $\frac{a3}{4}$ while this points in reciprocal lattice are

$a^*=\frac{a}{2}(1,1,-1)$

$b^*=\frac{a}{2}(1,-1,1)$ (2.1)

$c^*=\frac{a}{2}(-1,1,1)$

The reciprocal lattice of face centered cubic is body centered cubic and the first Brillion zone of FCC

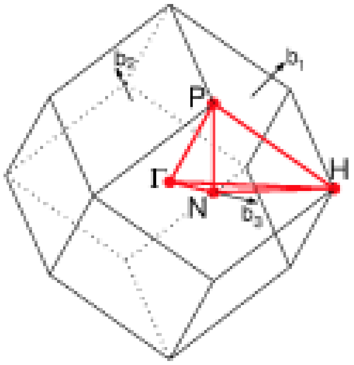


Figure 2.2: Brillion zone of BCC lattice. Path: Γ-H-N-Γ-P-H|P-N.

Table 2.2: Symmetry k-points of BCC lattice.

b_1	b_2	b_3		b_1	b_2	b_3	
0	0	0	Γ	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	P
$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	H	0	0	$\frac{1}{2}$	N

(Setyawan & Curtarolo., 2010)

2.2 Density functional theory (DFT)

DFT is a phenomenally successful approach for finding solutions to the fundamental equation of Schrödinger equation that describes the quantum behavior of atoms and molecules. Because Schrödinger equation is partial differential equation describing the quantitative behavior of any physical system and used to find the allowed energy level of quantum mechanical systems.DFT cancalculate the energy of a group of atoms or molecules and the density of electrons in the orbits in the quantum systems and gives excellent results and change the wave function that content 3Nvariables system to one body system. The time independent Schrödinger equation can be written as

$$\frac{-\hbar^2 \nabla^2}{2m\Psi(r)} + V(r)\Psi(r) = i \hbar \frac{\partial \Psi(r)}{\partial t} \qquad (2.2)$$

Where M is mass of the electron and Ψ(r) has no physical interpretation, the square of its absolute magnitude $|\Psi|^2$ evaluated at a particular place at a particular time is proportional to the probability of finding the body there at the time. When applying Schrödinger equation to calculate the $CeCrO_3$, which consists of electrons and nucleus, the term of kinetic energy in Schrödinger equation contains boththekinetic energy of the electrons and nucleus.

$$\text{Kinetic energy} = -\Sigma_{i=1} \frac{h^2 \nabla^2}{2me_i} - \Sigma_{I=1} \frac{h^2 \nabla^2}{2M_I} \qquad (2.3)$$

The potential energy term: $= \frac{e^2}{4\pi\varepsilon d_{ee}}$

$$(potentialenergy)ee = \frac{1}{2} \Sigma_{i \neq j} \frac{e^2}{4\pi\varepsilon} . \frac{1}{|r_i - r_j|}$$

The coulomb repulsion between electron pairs: $E_{nn} = \frac{z_I z_J}{4\pi\varepsilon d_{en}}$

$$(potentialenergy)nn = \frac{1}{2} \Sigma_{i \neq j} \frac{e^2}{4\pi\varepsilon} . \frac{z_I z_J}{|R_I - R_J|}$$

The coulomb repulsion between pairs of nuclei: $E_{en} = -\frac{2ze^2}{4\pi\varepsilon d_{en}}$

$$(potentialenergy)en = -\Sigma_{i \neq j} . \frac{z_I}{|r_i - R_I|}$$

We can rewrite the many-body Schrödinger equation as

$$\left| -\Sigma_{i=1} \frac{h^2 \nabla^2}{2me_i} - \Sigma_{I=1} \frac{h^2 \nabla^2}{2M_I} + \frac{1}{2} \Sigma_{i \neq j} \frac{e^2}{4\pi\varepsilon} . \frac{1}{|r_i - r_j|} + \frac{1}{2} \Sigma_{i \neq j} \frac{e^2}{4\pi\varepsilon} . \frac{z_I z_J}{|R_I - R_J|} - \Sigma_{i,j} \frac{e^2}{4\pi\varepsilon} . \frac{z_I}{|r_i - R_I|} \right| \Psi$$

$$= E_{tot} \Psi \qquad (2.4)$$

For solving equation (2.4) there are many type of approximation within DFT.

2.2.1 Types of DFT approximations:

The approximations within DFT are the following.

- Born-Opponheimer Theory
- Hohenberg Theory
- Kohn-Sham Equations

These approximation will be discussed in next points.

- **Born-Opponheimer Theory**

Let us consider any system that describe the properties of collection of atoms or molecule defining the crystal of an interesting mineral. The fundamental things we must know about this atoms or molecule are their energy and more importantly how this energy change sif we move the atoms around it.

In quantum mechanics we consider moving of the atoms as electrons and nucleus. Electron move rapidly than nuclei. In Born-Opponenheimerapproximation, the kinetic and potential energy of the nucleus can be neglected because they are too small for electrons energy. Thus, the Schrödinger equation

$$| -\Sigma_{i=1} \frac{h^2\nabla^2}{2me_i} + \frac{1}{2}\Sigma_{i\neq j} \frac{e^2}{4\pi\varepsilon}.\frac{1}{|r_i-r_j|} - \Sigma_{i,j} \frac{e^2}{4\pi\varepsilon}.\frac{z_I}{|r_i-R_I|}|\Psi = E_{tot}\Psi \qquad (2.5)$$

$\Psi(r_1,\ldots\ldots,r_N)$ is wavefunction of N electron, the probability is equal to $\Psi(r_1,\ldots\ldots,r_N)\ \Psi^*(r_1,\ldots\ldots,r_N)$ then the density of electrons at position r can be written

$$n(r) = 2\Sigma_i\ \Psi_i(r)\Psi_i^*(r) \qquad (2.6)$$

where n(r) is density of electrons in three coordinates. The factor 2 appear because Pauli Exclusion Principle(SHOLL & STECKEL., 2009).

- **Hohenberg Theory**

To formula density functional theory as an exact theory of many body systems

$$v_{ext}(r) \text{------} \square_i(r) \text{------} \Psi_0(r) \text{-----} n_0(r) \qquad (2.7)$$

External potential v_{ext}(r) determines all states of the systems $\square_i$(r), including the ground state Ψ_0(r) and ground state density n_0(r). The external potential involved any problem of electrons and fixed nuclei where the Hamiltonian of systems

$$-\sum_{i=1}\frac{h^2\nabla^2}{2me_i}+\frac{1}{2}\sum_{i\neq j}\frac{e^2}{4\pi\varepsilon}.\frac{1}{|r_i-r_j|}+v_{ext}(r)=H \tag{2.8}$$

Hohenberg theory consists of two theorem.

Theorem 1:

The external potential v_{ext}(r) and hence the total energy is unique functional of the electron density n(r).

$$E(n(r)) =< \Psi \,|\, H \,|\, \Psi^*> \tag{2.9}$$

Theorem 2:

The ground state energy can be obtained variationally: the density that minimizes the total energy is the exact ground state density.

$$E(n(r)) < E(n`(r)) \tag{2.10}$$

$$E_1^0+E_2^0 < E_2^0+E_1^0 \tag{2.11}$$

Hohnberg theory cannot successfully compute the ground state and density of electron in ground state by accurate way. Hohnberg only determined the ground state properties but cannot able to determine the ground state density and energy(Clark, The Hohenberg-Kohn Theorems, 2003).

- **Kohn-Sham approximation**

Kohn-Sham involved the exchange correlation functional to replace many body system to particle system. The energy functional can be written

$$E(\square_i(r)) = E_{known}(\square_i(r)) + E_{xc}(\square_i(r))$$

$$\left(-\frac{h^2\nabla^2}{2me_i}+V_n(r)+V_H(r)+V_{xc}(r)\right)\Psi=E_{tot}\Psi \tag{2.12}$$

Equation(2.12) is called Kohn-sham equations. Kohn-Sham equation changed many body system to single electron wave functions. The exchange correlation potential is V_{xc} (r) = $\frac{\delta E_{xc}(n)}{\delta n(r)}$, which is exchange and correlation contributions to the single electron equations.

To solve the single wavefunction of Khon-Sham equation there are many approximation that can be used. We will discuss the local density approximation sand generalized gradient approximation(SHOLL & STECKEL., 2009).

- **Local density approximation (LDA)**

Local density approximation used to find solution for the exchange correlation potential in Kohn-Sham equations. The exchange correlation energy is E_{xc}^{LDA}per electron density n(r). The density can be treated locally as an uniform electron gas, the exchange correlation energy at each point in an uniform electron gas the same density.

$$E_{xc}^{LDA} = \int n(r)\, \varepsilon_{xc}(n)\, dr \qquad (2.13)$$

ε_{xc} = exchange-correlation energy per particle of an uniform electron gas of density n(r). The exchange-correlation potential is given by

$$V_{xc}(r) = \frac{\delta E_{xc}(n)}{\delta n(r)} = \varepsilon_{xc}(n) + n(r)\frac{\partial \varepsilon_{xc}(n)}{\partial n(r)} \qquad (2.14)$$

$$\varepsilon_{xc}(n) = \varepsilon_{x}(n) + \varepsilon_{c}(n) \qquad (2.15)$$

and the exchange energy by Dirac functional

$$\varepsilon_{x}(n(r)) = -\frac{3}{4}\left(\frac{3}{\pi}\right)^{1/3} n(r) \qquad (2.16)$$

- **Generalized Gradient Approximation (GGA)**

Generalized gradient approximation is the best class of functional after local density approximation uses information about the local electron density and the local gradient in the electron density. It is content more physics information than LDA so this it is more accurate and also include two type of Perdew-Wang functional (PWA) and Perdew –Burke- Ernzerhof functional (PBE).

$$E_x[n]=\int(\boldsymbol{r})\varepsilon_{xc}(n(\boldsymbol{r}),\nabla n(\boldsymbol{r}))d\boldsymbol{r} \qquad (2.17)$$

(Martin, 2004)

2.3 Band Structure

In solid state physics, band gap of each material describe the range of energies that an electron may be have (allow zones) and it may be not have (forbidden zones). It depends on chemical and physical properties especially that is associated by atomic structure and atomic crystal. The band structure features break down the material into insulators, semiconductors and metal according to the band gap. Therefore one can define the band gap as the region between valance and conduction band.

2.4 Density of states

The density of state defined as the number of states per an interval of energy at each energy level available to be occupied. Density of state for valance and conduction band depend on states that are available for occupation and probability occupancy at that energy according to the pauli̓s exclusion.

2.5 Magnetic properties

- Magnetism is the phenomenon to describe how materials respond to magnetic field.
- Magnetic dipoles: magnetic forces are generated by moving electrically charged particles.
- Magnetic moments

It is the macroscopic magnetic properties of materials associated with spin motion of electrons and also it called magnetic dipole moments. Each in an atom has magnetic moment that originate from two source. One is the orbital motion around nucleus; electron behaves as small current loop, generating small magnetic field, and having a magnetic moment along it is axis of rotation. Another source is the orbital motion around itself; spin magnetic moment may be only in an up (parallel) direction or down (antiparallel) direction, generating small magnet having permanent orbitals and spin magnetic moments.

- Bohr magneton μ_B

It is the most fundamental magnetic moment, which magnitude is 9.27 x 10^{-24} A.m^2. For each electron in an atom the spin magnetic moment is + μ_B for spin up and - μ_B for spin down.

2.5.1 Types of magnetism

- Diamagnetic

This class of material is very weak form of magnetism. When an applied magnetic field leads change in orbital motion of electron, magnitude of magnetic moment is very small and in a direction opposite to that of the applied field and magnetic susceptibility is negative. In absence of an external field no dipole exists.

- Paramagnetic

This class of material until in an absence external field the atomic dipole are free to rotate. When applied external, the magnetic moment in same direction to that of the applied field and magnetic susceptibility is positive. Both diamagnetic and paramagnetic material are considered to be nonmagnetic because they exhibit magnetization only when the presence of an external field.

- Ferromagnetic

This certain metallic materials has permanent magnetic moments very strong interaction. This interaction produced by electronic exchange force and parallel or antiparallel alignment even an absence external field. It is has two characteristic is spontaneous magnetization and magnetic ordering temperature. Exchange force is very large, which is quantum mechanical phenomenon due to the relative orientation of the spins.

- Antiferromagnetic

This materials possesses sub lattice moments are exactly equal but opposite, so the net moments is zero.

This materials have magnetic moment coupling between adjacent atoms or ions occurs in materials other than those that are ferromagnetic. And possesses opposing magnetic moments cancel one another, and, as a consequence possesses net moments is zero.

- Ferrimagnetic

This material exhibit some ceramic also permanent magnetization and magnetic properties of ferromagnetic and ferromagnetic are similar so that are mean have net magnetic moments. The principle of ferromagnetism are illustrated with the cubic ferrites.

The cubic ferrites have the inverse spinel crystal structure, which is cubic symmetry, and similar to spinel structure (CALLISTER & JR., 1985,1991). To explain spinel structure check (section 13.2) from reference above.

Chapter Three

Material and Method

3.1 Introduction:

In this chapter, the simulation software by using quantum espresso software based on density functional theory (DFT), plane wave (PWSCF) and pseudo-potential (P.P) in ground state energy level were discussed. The numerical result of electronic and magnetic properties of perovskite compound $CeCrO_3$ was performed.

3.2 Quantum ESPRESSO (QE):

Quantum espresso is a software suite of electronic structure calculation, simulation, optimization and materials modeling based on density functional theory(DFT), plane wave(PW) basis sets and pseudo potential(PP) (both norm-conserving and ultra-soft). It is stands open source package for research in electronic structure, simulation and optimization. It is freely available to researchers around the world under the term of GNU general public license (GPL). Also we can say quantum espresso is computation technique for first principle calculation of periodic as well as disordered system. It calculates ground state energy, can be used to study metal, semiconductor and insulator.

Three main compound of method are PWSCF (plane wave self-consistent field), CP (Car Parinello), FPMD(first principle molecular dynamic) (Paolo Giannozzi, 2009).

3.2.1 PWSCF:

It is method to study the stability of crystal via density functional theory. It uses program of quantum espresso to calculation electronic structure that treated the electrons as waves. This waves are represent plane wave in two dimension corresponding wavefunction. One of programs that were used plane wave is PWSCF (plane wave self-consistent field) which can do particular in ground state energy, one electron (Kohn Sham) orbital, atomic forces, stresses structure optimization and also with variable cell.

3.2.2 Pseudo-potential:

Pseudo-potential or effective potential is an approximation for the simplified description of complex systems that is include atomic physics and neutron scattering. Pseudo-potential replace coulomb potential because it treated within core electrons in an uncomplicated way and there are two type of pseudo-potential namely, ultra-soft pseudo-potential and norm conserving pseudo-potential.

3.3.3 Exchange-correlation potential:

Exchange correlation potential is the function act to transform many body system to single electron wavefunction and we can be find solution of this function across LDA and GGA approximations (SHOLL & STECKEL., 2009).

3.4 General structure:

The input file of quantum espresso consists of:

- &Control:

It contents of the general variables controlling to run, i.e, type of calculation, prefix, restarte_mode, tstress, pseudo and outdir.

- &System:

It contents of the structural information on the system under investigation, i.e, ibrave, celldm, nat, ntyp, ecutwfc, ecutrho, occupation, nspin and starting magnetization.

- &Electrons:

It contents of the electronic variable, i.e, digonalization, mixed-beta and conv-thr.

- &Ions:

It is optional, content ionic variables, but in calculation of relax and vc-relax must be put in an input file.

- & Cell parameters:

It is optional, content dimension of crystal that it is represent by a, b, c, but must be exists if we choice ibrave is zero.

- &Cell:

It is optional, content variable cell dynamics, but in calculation of vc-relax exists in an input file.

- &Atomic species:

It is contents of the atomic symbol of any ntyp and atomic weight.

- &Atomic position:

It is contents of the atomic symbol and atomic position in unit cell according to date basis for any number of atoms.

- &K points:

K-point selection “automatic” tells PWSF to automatically generate k-point gird. Basic on nkx, nky, nkz, offx, offy, offz. Where nk number of interval in a direction and off offset of the origin of the gird.

Many physical and chemical properties of the materials can be calculated by using DFT methods. For our compound, band structure of the no magnetic and ferromagnetic properties were calculated (utility, 2019).

3.5 Method

In this study, predicated results were obtained by carrying the DFT which is quantum mechanic approach that successful predicating fundamental properties of compounds and alloys in term of semiconducting trend. In order to determine the ground state factor like lattice constant, we used GGA functional by considering the exchange –correlation potential suggested by Perdew, Burke and Ernzerh of (PBE). A mesh of 8x8x8 K-points was used irreducible part of the Brillion zone(BZ) for structural and electronic band properties, which certifies the convergence, are 60 K-points, for cubic CeCrO3 perovskites , the values were calculated to be 7.29 and 7.43a.u. (atomic units) for $CeCrO_3$. for energy convergence, the calculation of self-consistent were performed.

Chapter Four

Results

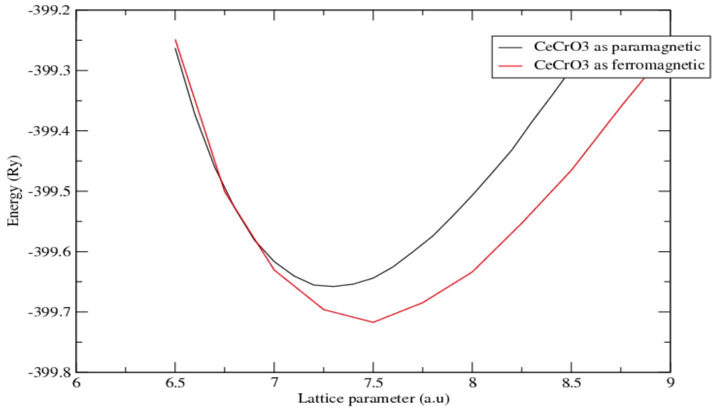
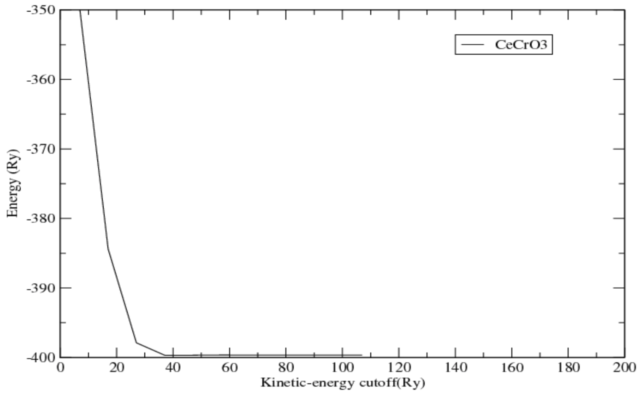


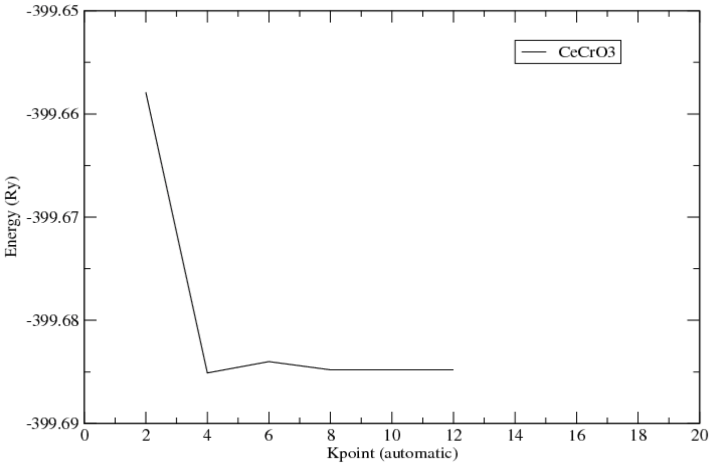
Figure (4.1):

Figure (4.1): shows the relationship between lattice parameter (a.u) and energy of ground state level (Ry) as paramagnetic and ferromagnetic.



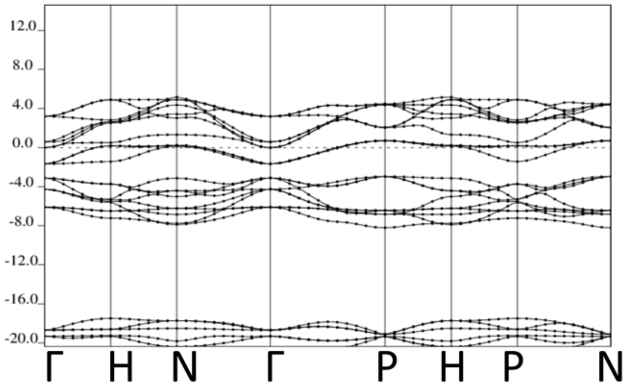
Figure(4.2):

Figure (4.2): shows relationship between energy (Ry) and kinetic energy cutoff (Ry) of $CeCrO_3$ as paramagnetic.



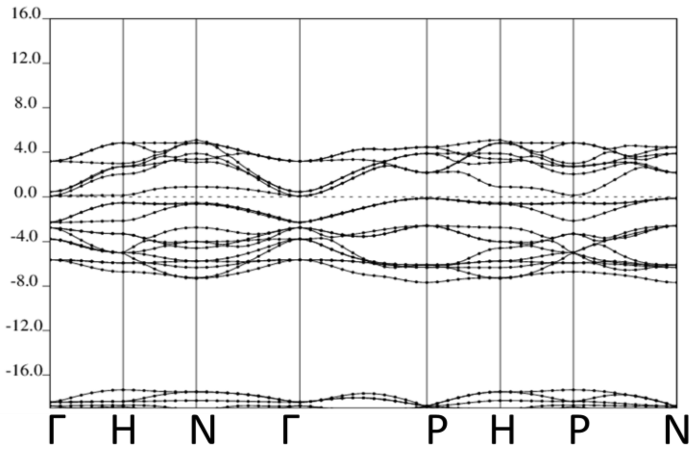
Figure(4.3):

Figure (4.3): shows relationship between energy (Ry) and k-point (automatic) of $CeCrO_3$ as paramagnetic.



Figure(4.4a):

Figure (4.4 a): show relationship between band gap (ev) and k path of first Brillion zone(k-points) of $CeCrO_3$ as paramagnetic.



Figure(4.4b):

Figure (4.4 b): show relationship between band gap (eV) and k path of first Brillion zone(k-points) of $CeCrO_3$ as ferromagnetic.

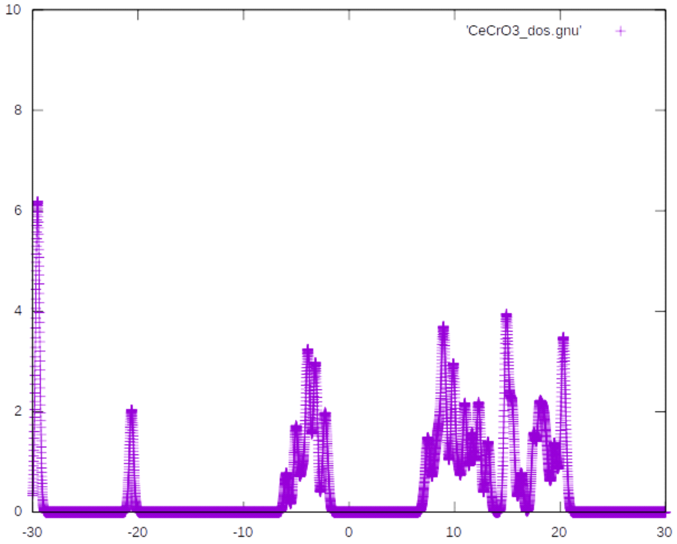


Figure (4.5 a):

Figure (4.5 a): show relationship between density of state (DOS) and energy (ev) of the $CeCrO_3$ as paramagnetic.

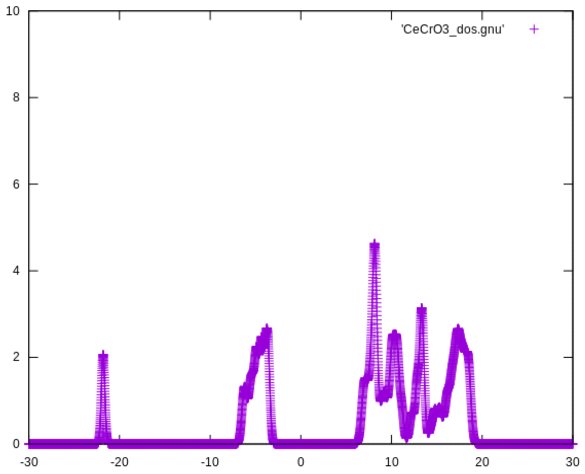


Figure (4.5 b):

Figure (4.5 b): show relationship between density of state (DOS) and energy (ev) of the $CeCrO_3$ as ferromagnetic.

Chapter Five

Discussion and Conclusion and Recommendation

5.1 Discussion:

In figure (4.1) were found that the energy is decreased with increasing the lattice parameter, at specific point the energy was increased. We can determine the lattice parameter accurately via fitting by using birch1 with method . The calculated lattice parameter was 3.86 Å for paramagnetic and 3.93 Å for ferromagnetic material respectively.

In order to perform real calculation of the electronic structure of our compound the following optimization was done. In figure(4.2) The energy is decreased rapidly with increasing the energy cut-off wavefunction but as some stage it is stabilized from 37 Ry. Therefore the value of 37 Ry was used for all calculations.

In figure (4.3) The energy is decreased rapidly with increasing the k-point (automatic) but as some stage it is stabilized from 8. Therefore the value of 8 was used for all calculations.

Figure(4.4a) and (4.4b): show relationship between band gap eV and k path of first Brillion zone(k-points) of $CeCrO_3$ as paramagnetic and ferromagnetic, values of each ones is 0.4 eV and 3.36 eV respectively. The different between two values due to spin of electron.

Figure (4.5 a) and (4.5 b) show relationship between density of state (DOS) and energy eV of the $CeCrO_3$ as paramagnetic and ferromagnetic with different magnetization. Therefore appear the density of state as ferromagnetic high than paramagnetic due to spins of electrons and magnetic moment aligned of $CeCrO_3$, so the net magnetization non zero.

5.2 Conclusion:

The electronic band structure of the $CeCrO_3$ crystal as paramagnetic and ferromagnetic were calculated. In order to performed real calculation for the band structure, the structural optimization of energy cut-off and K-point as well as lattice parameter were done. The lattice parameter were found to be 3.86 Å and 3.93 Å respectively and the band gap were 0.4 eV and 3.36 eV and appear the density of state as ferromagnetic high than paramagnetic as expected.

5.3 Recommendation:

In this study the electronic band structure of the CeCrO3 compound as paramagnetic and ferromagnetic were studied. Further examination of CeCrO3 compound as paramagnetic and ferromagnetic can be performed. The optical properties, transport properties and thermal properties of the compound are recommended for future work.

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