



بِسْمِ اللَّهِ الرَّحْمَنِ الرَّحِيمِ

Sudan University of Science and Technology (SUST)

College of Graduate Studies



**Effect of Magnetization on Ferrromagnetic and
Antiferromagnetic for NiO Properties Using Quantum
ESPRESSO Package**

تأثير المغنطة على خصائص أوكسيد النيكل الفيرومغناطيسية والفيرومغناطيسية المضادة
بإستخدام المحاكاة (Quantum ESPRESSO)

A thesis submitted in partial fulfillment of the Requirements for the
M.Sc. degree in Physics

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DEDICATION

I dedicate this research to my parents, my brother Mutasim, all my family, and all my best friends.

ACKNOWLEDGEMENTS

I would like to express my sincere and appreciation to my supervisor Dr. Abdelnabi Ali Elamin, for providing work facilities, for his kind guidance, science support, continuous encouragement in order to finish this work. From my deep heart, many thanks are paid to Dr. Arwa Algadal, U.Gamr Alanbya for suggesting the research point. Also, sincere thanks to all staff in the Department of Physics, Faculty of Science, Sudan University, for their encouragement.

ABSTRACT

The magnetic properties of NiO as ferromagnetic and antiferromagnetic behavior were studied as implemented in the quantum ESPRESSO package. From density of state curves it was observed that ferromagnetic materials have high density of state (DOS) than antiferromagnetic materials at the same value of magnetization. Also from band structure diagram found that there is no any difference between band gap of NiO as ferromagnetic and antiferromagnetic materials, It is direct band gap within quantum ESPRESSO.

المستخلص

تم دراسة الخواص المغناطيسية لأكسيد النيكل كمادة فيرومغناطيسية ومادة فيرومغناطيسية مضادة باستخدام حزمة المحاكاة Quantum ESPRESSO. من خلال منحنيات كثافة الحالات (DOS) لوحظ أنه عندما نتعامل مع أكسيد النيكل كمادة فيرومغناطيسية تكون كثافة الحالات عالية مقارنة بالسلوك الفيرومغناطيسي المضاد عند نفس قيمة المغنطة، وقد وجد ان طاقة مستوى فيرمي (E_F) لأكسيد النيكل كمادة فيرومغناطيسية أكبر من الفيرومغناطيسية المضادة له مع تغير قيمة المغنطة، ايضا من منحنى نطاق الطاقة وجد أنه لا يوجد فرق بين فجوة الطاقة لأكسيد النيكل عندما يكون مادة فيرومغناطيسية او فيرومغناطيسية مضادة.

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Chapter 1

Introduction

1.1 Introduction

In solid state physics, the electronic band structure (or simply band structure) of a solid describes the range of energies that an electron within the solid may have (called energy bands, allowed bands, or simply bands) and ranges of energy that it may not have (called band gaps or forbidden bands). Band theory derives these bands and band gaps by examining the allowed quantum mechanical wave functions for an electron in a large, periodic lattice of atoms or molecules. Band theory has been successfully used to explain many physical properties of solids, such as electrical resistivity and optical absorption, and forms the foundation of the understanding of all solid state devices (transistors, solar cells, etc). Band structure calculations take advantage of the periodic nature of a crystal lattice, exploiting its symmetry[1].

The density of states function $g(E)$ is defined as the number of electronic states per unit volume, per unit energy, for electron energies near (E) . The density of states function is important for calculations of effects based on band theory. It appears in calculations for optical absorption where it provides both the number of excitable electrons and the number of final states for an electron. It appears in calculations of electrical conductivity where it provides the number of mobile states, and in computing electron scattering rates where it provides the number of final states after scattering[1].

Computer simulations are nowadays an integral part of contemporary basic and applied research in the sciences. Computation is becoming as important as theory and experiment. In physics, computational physics, theoretical physics and experimental physics are all equally important in our daily research and studies of physical systems. Physics is the unity of theory, experiment and computation. Moreover, the ability "to compute" forms part of the essential repertoire of research scientists. Several new fields within computational science have emerged and strengthened their positions in the last years, such as computational materials science, computational mathematics and mechanics, computational chemistry and physics and so forth, just to mention a few. These fields underscore the importance of simulations as a means to gain novel insights into physical systems, especially for those cases where no analytical solutions can be found or an experiment is too complicated or expensive to carry out. To be able to simulate large quantal systems with many degrees of freedom such as strongly interacting electrons in a quantum dot will be of great importance for future directions in novel fields like nano technology. This ability often combines knowledge from many different subjects, in our case essentially from the physical sciences, numerical mathematics, computing languages, topics from high performance computing and some knowledge of computers [2].

The Nickel oxide (NiO) has a fcc crystal structure with two atoms in the unit cell. The Ni atoms spin polarize and form an antiferromagnetic arrangement in the (111) direction of the fcc cell. The structure can be described by a Rhombohedral unit cell with 4 atoms in the basis [3]. NiO

has a variety of specialized applications and generally applications distinguish between “chemical”, which is relatively pure material for specialty applications, It is used in the ceramic industry to make first, ferrites and porcelain glazes. The sintered oxide is used to produce nickel steel alloys, NiO was also a component in the nickel iron battery, also known as the Edison Battery, and is a component in fuel cells It is the precursor to many nickel salts, for use as oxide. and catalysts. More recently, NiO quality annually, mainly as an intermediate in the product was used to make the NiCd rechargeable batteries found in many electronic devices [4].

1.2 Problem of Research

Setup of laboratory experiments require materials, accurate devices and an environment fit experience, this is expensive financially, spatially and requires a great time until we get the results, so it was necessary to find a solution is to use simulation software, where we find that it is inexpensive and requires less time and can be used for predictions.

1.3 Objectives of Research

The objectives of research are calculation and compare of some parameters for NiO such as : density of state, Fermi Energy, enregy gap, Band tructure for antiferromagnetic material and ferromagnetic material at variable values of magnetization.

1.4 Lay out of Reseach

A thesis contains four chapters, the first chapter contains an introduction to research and objectives of research in addition to the research problem, either in Chapter two spoke of nickel oxide and how to

prepare it, its various applications, its properties and then addressed the magnetic properties in general and its relationship with the crystal structure, in Chapter Three touched upon the simulation software and how to use the data entry, the fourth chapter deals with the findings through research and interpretation of the results, Discussion, Conclusions and document references.

Chapter 2

Magnetic Materials

2.1 Introduction

Magnetic materials encompass a wide variety of materials, which are used in a diverse range of applications. Magnetic materials are utilized in the creation, distribution of electricity and in most cases in the appliances that use that electricity. They are used for the storage of data on audiotape and videotape and on computer disks. In the world of medicine, they are used in body scanners and in a range of applications where they are attached to or implanted into the body. The home entertainment market relies on magnetic materials in applications such as CD players, televisions, games consoles, and loudspeakers.

Magnetic materials are classified in terms of their magnetic properties and their uses. If a material is easily magnetized and demagnetized then it is referred to as a soft magnetic material, whereas if it is difficult to demagnetize then it is referred to as a hard (or permanent) magnetic material. Materials in between hard and soft are almost exclusively used as recording media and have no other general term to describe them. Other classifications for types of magnetic materials are subsets of soft or hard materials.

2.2 Magnetic Terminology and Units

In the study of magnetism there are two systems of units currently in use : the mks(metres, kilograms, seconds) system, which has been adopted as the S.I units and the cgs (centimeters, grams, seconds) system, which is

also known as the Gaussian system. The cgs system is used by many magnets experts because of the numerical equivalence of the magnetic induction (B) and the applied field (H). When a field is applied to a material then it responds by producing a magnetic field, the magnetization (M). This magnetization is a measure of the magnetic moment per unit volume of material, but can also be expressed per unit mass and is called the specific magnetization (σ). The field that is applied to the material is called the applied field (H) and is the total field that would be present if the field were applied to a vacuum. Another important parameter is the magnetic induction (B), which is the total flux of magnetic field lines through a unit cross sectional area of the material, considering both lines of force from the applied field and from the magnetization of the material. B, H, and M are related by eq. (2.1) in S.I. units and by Eq. (2.2) in cgs units.

$$B = \mu_0 (H + M) \quad (2.1)$$

$$B = H + 4 \pi M \quad (2.2)$$

In eq. (2.1), the constant μ_0 is the permeability of free space ($4\pi \times 10^{-7} \text{ H.m}^{-1}$), which is the ratio of B/H measured in a vacuum. In cgs units the permeability of free space is unity and so does not appear in eq. (2.2).

Another equation (eq. (2.3), the same for S.I. and cgs units) to consider at this stage is that concerning the magnetic susceptibility (χ), which is a parameter that demonstrates the type of magnetic material and the strength of that type of magnetic effect.

$$X = M/H \quad (2.3)$$

Sometimes the mass susceptibility (X_m) is quoted and this has the units of

$\text{m}^3 \text{kg}^{-1}$ and can be calculated by dividing the susceptibility of the material by the density.

Another parameter that demonstrates the type of magnetic material and the strength of that type of magnetic effect is the permeability (μ) of a material, which is defined in eq. (2.4).

$$\mu = B/H \quad (2.4)$$

In the S.I. system of units, the permeability is related to the susceptibility, as shown in eq. (2.5) and can also be broken down into μ_r and the relative permeability (μ_r), as shown in Eq. (2.6).

$$\mu = \chi + 1 \quad (2.5)$$

$$\mu = \mu_0 \cdot \mu_r \quad (2.6)$$

Finally, an important parameter (in S.I. units) to know is the magnetic polarization (J), sometimes referred to as the intensity of magnetization (I). This value is effectively the magnetization of a sample expressed in Tesla, and can be calculated as shown in eq.(2.7).

$$J = \mu_0 \cdot M \quad (2.7)$$

2.3 Types of Magnetic material

2.3.1 Diamagnetism

In a diamagnetic material the atoms have no magnetic moment when there is no applied field. Under the influence of an applied field (H) the spinning electrons precess, and this motion, which is a type of electric current, produces a magnetization (M) in the opposite direction to that of the applied field. All materials have a diamagnetic effect. However, in non diamagnetic material another effect makes the diamagnetic contribution

insignificant. The value of susceptibility is independent of temperature.

2.3.2 Paramagnetism

There are several theories of paramagnetism, which are valid for specific types of material. The Langevin model, which is true for materials with noninteracting localized electrons, states that each atom has a magnetic moment which is randomly oriented as a result of thermal agitation. The application of a magnetic field creates a slight alignment of these moments and hence a low magnetization in the same direction as the applied field. As the temperature increases, then the thermal agitation will increase and it will become harder to align the atomic magnetic moments and hence the susceptibility will decrease. This behavior is known as the Curie law and is shown below in eq. (2.8), where C is a material constant called the Curie constant.

$$X = C/T \quad (2.8)$$

Materials that obey this law are materials in which the magnetic moments are localized at the atomic or ionic sites and where there is no interaction between neighboring magnetic moments. The hydrated salts of the transition metals, e.g., which have a magnetic moment, are surrounded by a number of nonmagnetic ions / atoms, which prevent interaction between neighboring magnetic moments. In fact the Curie law is a special case of the more general Curie-Weiss law, eq. (2.9), which incorporates a temperature constant (θ) and derives from Weiss theory which incorporates the interaction between magnetic moments.

$$X = C/(T - \theta) \quad (2.9)$$

In this equation, θ can either be positive, negative, or zero. Clearly when ($\theta = 0$) then the Curie-Weiss law equates to the Curie law. When θ is nonzero then there is an interaction between neighboring magnetic moments, and the material is only paramagnetic above a certain transition temperature. If θ is positive, then the material is ferromagnetic below the transition temperature, and the value of θ corresponds to the transition temperature (Curie temperature, T_C). If θ is negative then the material is anti ferromagnetic below the transition temperature (Néel temperature, T_N). However the value of θ does not relate to T_N . It is important to note that this equation is only valid when the material is in a paramagnetic state. It is also not valid for many metals, as the electrons contributing to the magnetic moment are not localized. However, the law does apply to some metals, e.g. the rare earths, where the 4f electrons, which create the magnetic moment, are closely bound.

The Pauli model of paramagnetism is true for materials where the electrons are free and interact to form a conduction band and is valid for most paramagnetic metals. In this model the conduction electrons are considered essentially to be free, and under an applied field an imbalance between electrons with opposite spin is set up leading to a low magnetization in the same direction as the applied field. The susceptibility is independent of temperature, although the electronic band structure may be affected, which will then have an effect on the susceptibility.

2.3.3 Ferromagnetism

Ferromagnetism is only possible when atoms are arranged in a lattice and the atomic magnetic moments can interact to align parallel to each

other. This effect is explained in classical theory by the presence of a molecular field within the ferromagnetic material, which was first postulated by Weiss in 1907. This field is sufficient to magnetize the material to saturation. In quantum mechanics, the Heisenberg model of ferromagnetism describes the parallel alignment of magnetic moments in terms of an exchange interaction between neighboring moments.

Weiss postulated the presence of magnetic domains (considered later) within the material, which are regions where the atomic magnetic moments are aligned. The movement of these domains determines how the material responds to a magnetic field and as a consequence the susceptibility is a function of applied magnetic field. Therefore, ferromagnetic materials are usually compared in terms of saturation magnetization (magnetization when all domains are aligned) rather than susceptibility.

In the periodic table of elements only Fe, Co, and Ni are ferromagnetic at and above room temperature. As ferromagnetic materials are heated, the thermal agitation of the atoms means that the degree of alignment of the atomic magnetic moments decreases and hence the saturation magnetization also decreases.

2.3.4 Antiferromagnetism

In the periodic table the only element exhibiting antiferromagnetism at room temperature is chromium. Antiferromagnetic materials are similar to ferromagnetic materials, but the exchange interaction between neighboring atoms leads to the antiparallel alignment of the atomic magnetic moments. Therefore, the magnetic field cancels out, and the material appears to

behave in the same way as a paramagnetic material. Like ferromagnetic materials these materials become paramagnetic above a transition temperature, known as the Néel temperature, T_N . (Cr : $T_N = 37^\circ\text{C}$).

2.3.5 Ferrimagnetism

Ferrimagnetism is only observed in compounds, which have more complex crystal structures than pure elements. Within these materials the exchange interactions lead to parallel alignment of atoms in some of the crystal sites and antiparallel alignment of others. The material breaks down into magnetic domains, just like a ferromagnetic material, and the magnetic behavior is also similar, although ferrimagnetic materials usually have lower saturation magnetizations.

2.3.6 The saturation magnetization (M_S)

The saturation magnetization (M_S) is a measure of the maximum amount of field that can be generated by a material. It will depend on the strength of the dipole moments on the atoms that make up the material and how densely they are packed together. The atomic dipole moment will be affected by the nature of the atom and the overall electronic structure within the compound. The packing density of the atomic moments will be determined by the crystal structure (i.e. the spacing of the moments) and the presence of any nonmagnetic elements within the structure.

For ferromagnetic materials, at finite temperatures, M_S will also depend on how well these moments are aligned, as thermal vibration of the atoms causes misalignment of the moments and a reduction in M_S . For ferrimagnetic materials not all of the moments align parallel, even at zero Kelvin and hence M_S will depend on the relative alignment of the

moments as well as on the temperature. The saturation magnetization is also referred to as the spontaneous magnetization, although this term is usually used to describe the magnetization within a single magnetic domain[5].

2.4 Information about NiO

Nickel(II) oxide is the chemical compound with the formula NiO. It is notable as being the only well characterized oxide of nickel (although nickel(III) oxide[6].

The mineralogical form of NiO, bunsenite, is very rare. It is classified as a basic metal oxide. Several million kilograms are produced in varying quantity annually, mainly as an intermediate in the production of nickel alloys[7].

2.4.1 Structure of NiO

NiO adopts the NaCl structure, with octahedral Ni(II) and O⁻² sites. The conceptually simple structure is commonly known as the rock salt structure. Like many other binary metal oxides, NiO is often non stoichiometric, meaning that the Ni:O ratio deviates from 1:1. In nickel oxide this non-stoichiometry is accompanied by a color change, with the stoichiometrically correct NiO being green and the non-stoichiometric NiO being black[8].

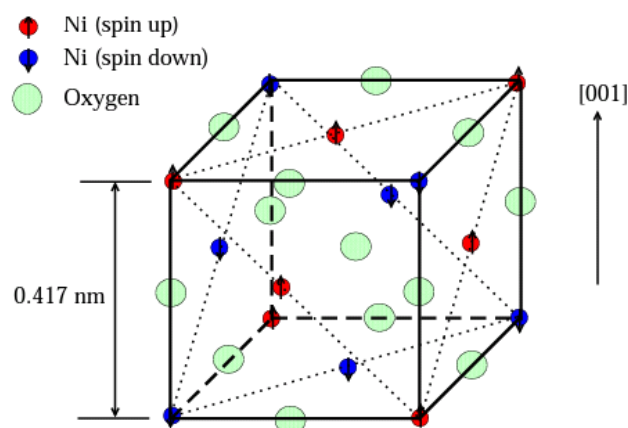
2.4.2 Theoretical outline

In QUASST (quantum atomistic solid state theory) the insulating ground state of NiO results from the ionic state Ni⁺² O⁻² . These ionic states are formed during the formation of the compound. One can also say that such charge redistribution results from

strong hybridization of $3d(\text{Ni})-2p(\text{O})$ states thanks which the nickel atoms are ready to give up two electrons and the oxygen atoms energetically prefer to accept these two electrons, becoming O^{-2} ions. The O^{-2} ions assume the full $2p\ 6$ configuration and are magnetically and energetically silent[9][10].

2.4.3 Magnetic propertise of NiO

NiO, one of the most favored antiferromagnets, is a prototypic system for strong electronic correlations with high spin AF_2 structure at low temperatures and has a simple crystallographic rock salt structure with a lattice constant of 0.417 nm (see Fig. 2.1). There are two components of spin configurations due to the non-local exchange interaction. For the first component, the direct exchange interaction between the nearest neighbour of Ni ions favors paring of spins to lower energy. For another one, a very strong interaction comes from the super exchange between the next nearest neighbour of Ni ions. This makes the antiferromagnetic spin structure for the ground state of NiO[11].



Fig(2.1): shows the structure of NiO AF_2 antifrromagnetic spin structure [11].

Chapter 3

Simulation software

3.1 Quantum ESPRESSO (QE)

Quantum ESPRESSO is an integrated suite of computer codes for electronic structure calculations and materials modeling, based on density-functional theory (DFT), plane waves (PW), and pseudopotentials (PP) (norm-conserving, ultrasoft, and projector-augmented wave).

Quantum ESPRESSO stands for opEn Source Package for Research in Electronic Structure, Simulation, and Optimization. It is freely available to researchers around the world under the terms of the GNU General Public License. Quantum ESPRESSO builds upon newly restructured electronic structure codes that have been developed and tested by some of the original authors of novel electronic-structure algorithms and applied in the last twenty years by some of the leading materials modeling groups worldwide. Innovation and efficiency are still its main focus, with special attention paid to massively-parallel architectures, and a great effort being devoted to user friendliness. Quantum ESPRESSO is evolving towards a distribution of independent and inter-operable codes in the spirit of an open-source project, where researchers active in the field of electronic structure calculations are encouraged to participate in the project by contributing their own codes or by implementing their own ideas into existing codes[12].

3.2 About Quantum Espresso

It is a computational technique for first principle calculation of periodic as well as disordered systems. It is mainly based on DFT theory (electron-ion interaction), plane wave and pseudopotentials (electron-electron interaction). It calculates the ground state energy and Kohn Sham orbital for both insulators and metals and various type of structural optimizations. Quantum espresso can be used to study metals, semiconductors as well as insulators.

Three main components of method are PWSCF (Plane wave self consistent field), CP (Car Parinello), FPMD (First principle molecular dynamics).

3.2.1 PWSCF

It is a method to calculate the phonon dispersions for complex materials,i.e., to study the stability of crystal. The electronic structures can be calculated by expanding the wavefunctions into planewaves.

3.2.2 Pseudopotential

It is a modified effective potential term instead of coulombic potential term in Schroedinger equation for core electrons. There are two types of Pseudopotentials,i.e, ultrasoft pseudopotential and Norm conserving pseudopotential. The information about the type of exchange co-relational functional and type of pseudopotential can be found from the name of pseudopotential. Plane wave formalism usually performed in combination with pseudopotential because a large number of plane waves are required to expand wavefunctions which is an obstacle to increase the

computational efficiency. In pseudopotential, the Kohn Sham's radial equation is considered. It contains the contribution from valence electrons.

3.2.3 Exchange Co-relation potential

Need to diagonalize a matrix by iterative method. The no of eigenvalue computed for metals depends on valence electron[13].

3.3 The Quantum ESPRESSO Software Distribution

The democritos center of Italian INFM is dedicated to atomistic simulations of materials, with a strong emphasis on the development of high quality scientific software. Quantum espresso is the result of a democritos initiative, in collection with several other institutions (ICTP, CINECA Bologna, MIT, Paris VI, Oxford and Princeton university) Quantum espresso is a distribution of software for atomistic simulations based on electronic structure ... etc .

3.4 License for quantum espresso

Quantum espresso is distributed under the GUN General public license (GPL), probably the most common free software license . Basicly :

- * the source code is available .
- * you can do whatever you want with the sources,

Advantages :

- * Every body _ including commercial entities _ can contribute .
- * Nobody can steal the code and give nothing back to the community[14].

Quantum ESPRESSO is an integrated suite of computer codes for electronic-structure calculations and materials modeling at the nanoscale.

3.5 Codes under Quantum ESPRESSO

- * PWSCF : Plane-wave self consistent field.

- * CP : Car-Parrinello molecular dynamics.
- * PHONON : Phonon calculations.
- * FPMD : Molecular Dynamics.

3.6 Capabilities

- * Self-consistent, planewave, pseudopotential total energy calculation.
- * Large xc library : LDA, GGA, BLYP, LDA+U.
- * Pseudopotential generation code and pseudopotential library Norm-conserving, ultrasoft.
- * Geometric optimization also with variable cells.
- * Phonon calculations, (harmonic/anharmonic/e-ph).
- * Inclusion of electric field, macroscopic polarizability.
- * Noncollinear magnetism.
- * Infrared and Raman cross sections.
- * Dielectric tensors.
- * Ballistic conductance.
- * Maximally localized Wannier functions.
- * Nudged Elastic Bands (NEB).

3.7 General structure

The input file is broken down into sections :

Namelist — calculation specifications

&CONTROL: general variables controlling the run.

&SYSTEM: structural information on the system under investigation.

&ELECTRONS: electronic variables.

&IONS (optional): ionic variables.

&CELL (optional): variable-cell dynamics.

&PHONON (optional): information required to produce data for phonon calculations.

3.8 General structure

Nonoptional and optional cards

* ATOMIC SPECIES : Atomic species for each ntyp enter atomic symbol atomic weight pseudopotential.

* ATOMIC POSITIONS : Atomic positions, for each nat enter atomic symbol x y z where x,y,z are given as fractional coordinates of the conventional cell.

* K POINTS : k-point selection “automatic” tells PWSCF to automatically generate a k-point grid. The format of the next line is nkx nky nkz offx offy offz, where nk* is the number of intervals in a direction and off* is the offset of the origin of the grid.

* CELL PARAMETERS(optional)

* OCCUPATIONS(optional)

* FIRST IMAGE(optional)

* LAST IMAGE(optional)

* CLIMBING IMAGES(optional)[15].

3.9 The input data of NiO as ferromagnetic material

self-consistent calculation

cat > nio_fm.scf.in << EOF

&control

prefix='nio',

&system

ibrav= 0, celldm(1)=7.93, nat= 4, ntyp= 3,

ecutwfc = 30.0, ecutrho = 300.0

nspin=2,

starting_magnetization(2)= 0.2 or 0.4 or 0.6,

starting_magnetization(3)=0.2 or 0.4 or 0.6,

CELL_PARAMETERS

0.50 0.50 1.00

0.50 1.00 0.50

1.00 0.50 0.50

ATOMIC_SPECIES

O 1. O.pbe-rrkjus.UPF

Ni1 1. Ni.pbe-nd-rrkjus.UPF

Ni2 1. Ni.pbe-nd-rrkjus.UPF

ATOMIC_POSITIONS crystal

O 0.25 0.25 0.25

O 0.75 0.75 0.75

Ni1 0.0 0.0 0.0

Ni2 0.5 0.5 0.5

K_POINTS automatic

4 4 4 0 0 0

EOF

\$bin/pw.x < nio_fm.scf.in > re_NiO_fm2/nio.scf.out

3.10 The input data of NiO as antiferromagnetic material

self-consistent calculation

cat > nio_fm.scf.in << EOF

&control

prefix='nio',

&system

ibrav= 0, celldm(1)=7.93, nat= 4, ntyp= 3,

ecutwfc = 30.0, ecutrho = 300.0,

nspin=2,

starting_magnetization(2)= 0.2 or 0.4 or 0.6,

starting_magnetization(3)= -0.2 or -0.4 or -0.6,

&electrons

CELL_PARAMETERS

0.50 0.50 1.00

0.50 1.00 0.50

1.00 0.50 0.50

ATOMIC_SPECIES

O 1. O.pbe-rrkjus.UPF

Ni1 1. Ni.pbe-nd-rrkjus.UPF

Ni2 1. Ni.pbe-nd-rrkjus.UPF

ATOMIC_POSITIONS crystal

O 0.25 0.25 0.25

O 0.75 0.75 0.75

Ni1 0.0 0.0 0.0

Ni2 0.5 0.5 0.5

K_POINTS automatic

4 4 4 0 0 0

EOF

\$bin/pw.x < nio_fm.scf.in > re_NiO_fm2/nio.scf.out

Chapter 4

Result and Discussion

From table (4.1) and fig (4.1) below , explains the changing of fermi energy with different value of magnetization, Also show the NiO as ferromagnetic material has larger Fermi energy (E_F) than antiferromagnetic, may be due to the spins of electrons and magnetic moments are aligned of NiO as ferromagnetic, So the net magnetization non zero.

Table (4-1): Magnetization and Fermi energy of NiO

| Value of magnetization(M) $A.m^{-1}$ | Fermi energy(E_F) eV of NiO as ferromagnetic | Fermi energy (E_F) eV of NiO as antiferromagnetic |
|--------------------------------------|--|---|
| 0.2 | 11.7873 | 11.3340 |
| 0.4 | 11.7884 | 11.3340 |
| 0.6 | 11.7881 | 11.336 |
| 0.8 | 11.7861 | 11.3339 |
| 1.0 | 11.7872 | 11.3344 |

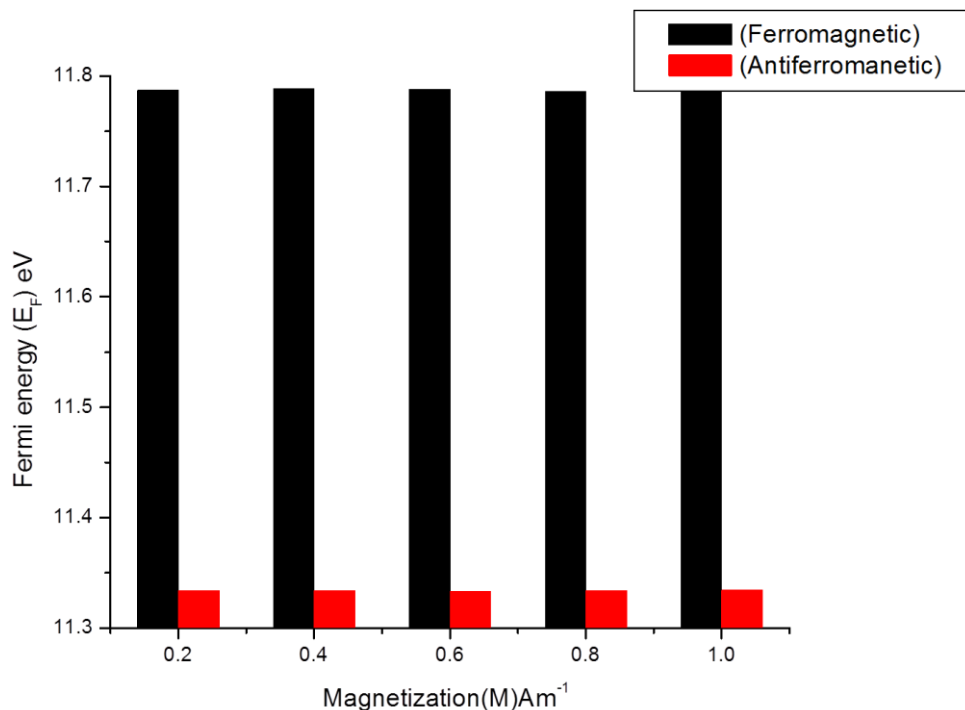
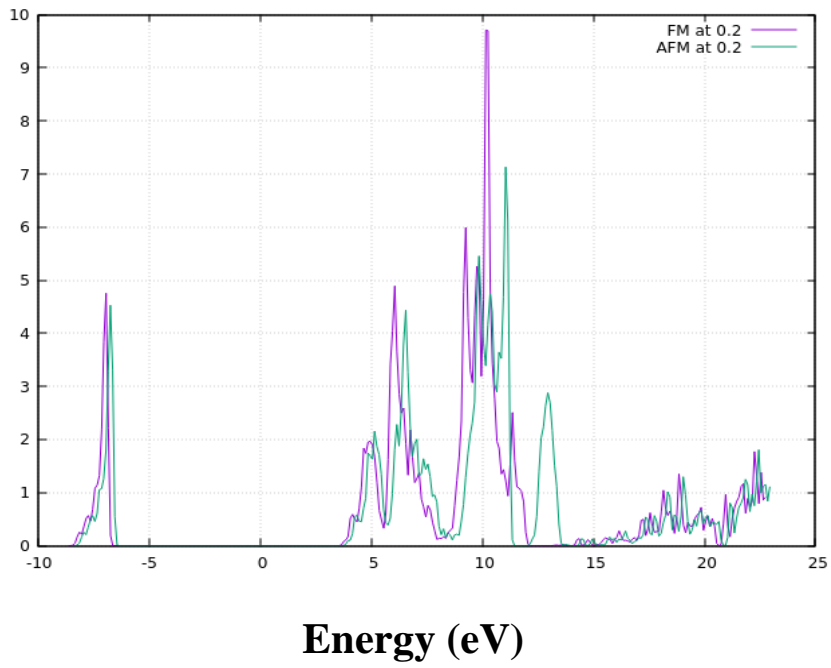


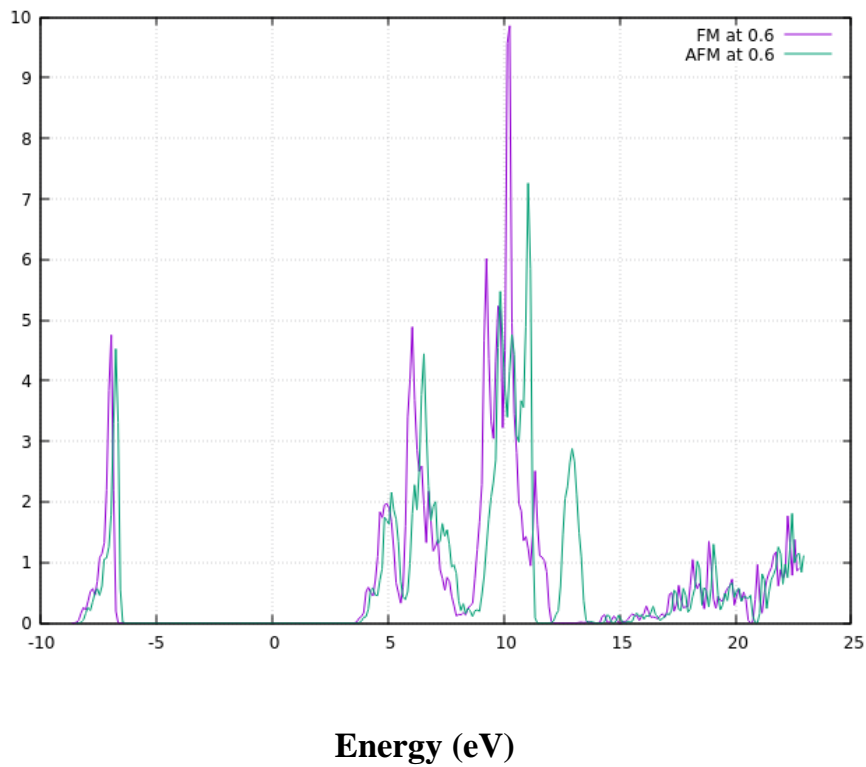
Table (4-1) and Fig (4-1) : shows the fermi energy (E_F) eV and magnetization(M) Am^{-1} curve of NiO as ferromagnetic and antiferromagnetic materials .

DOS



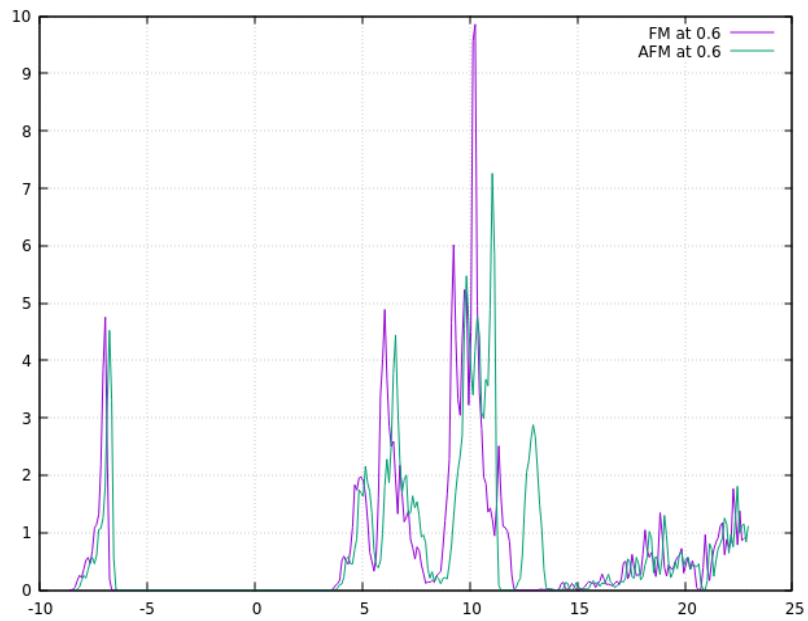
Fig(4-2) : shows density of state (DOS) and Energy (eV) of NiO as aferromagnetic and antiferromagnetic material at magnetization 0.2A.m^{-1} .

DOS



Fig(4-3) : shows density of state (DOS) and Energy (eV) curve of NiO as aferromagnetic and antiferromagnetic material at magnetization 0.4 A.m^{-1} .

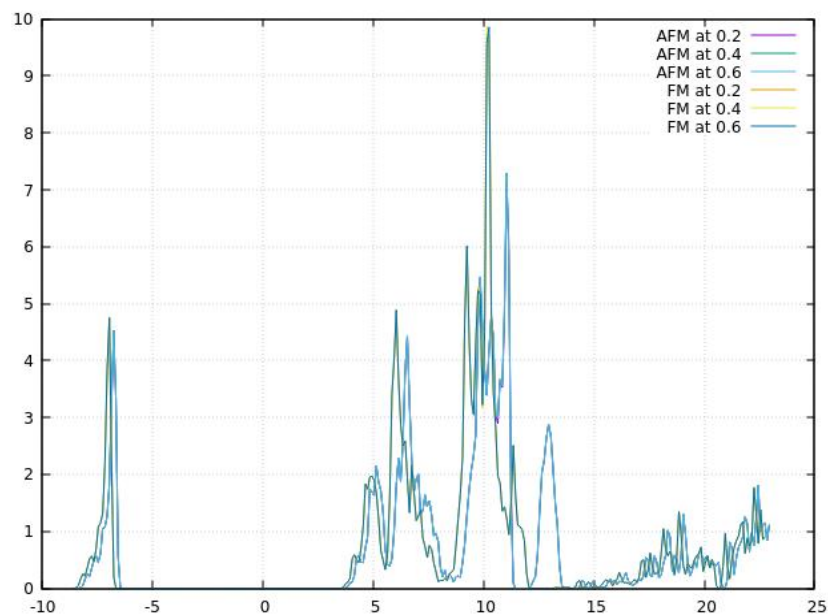
DOS



Energy (eV)

Fig(4-4) : shows density of state (DOS) and Energy (eV) curve of NiO as aferromagnetic and antiferromagnetic material at magnetization 0.6 A.m^{-1} .

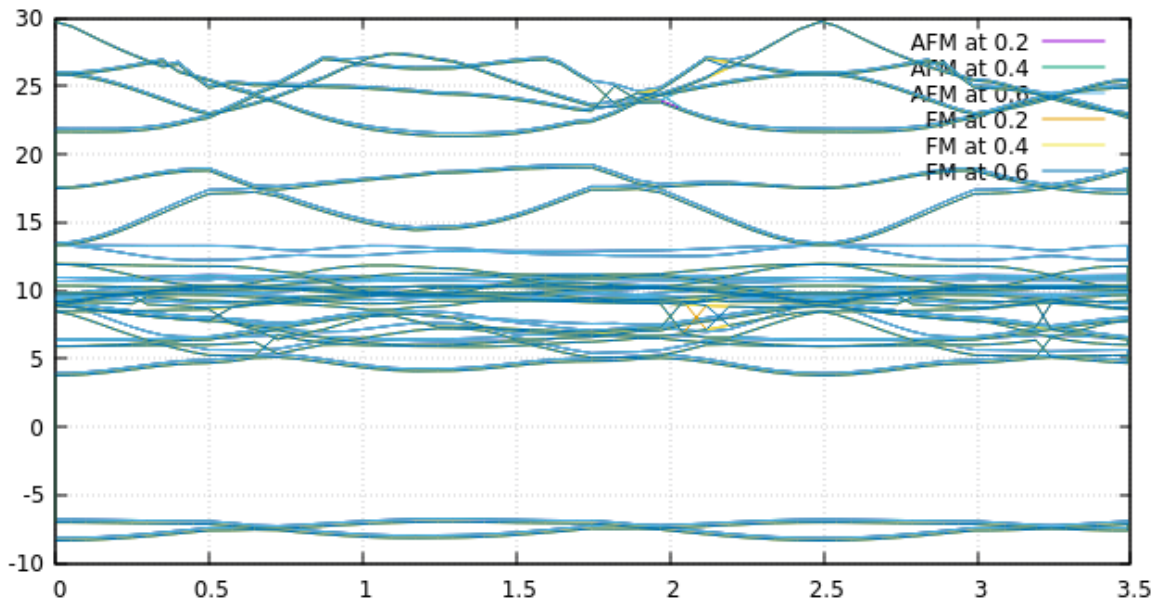
DOS



Energy (eV)

Fig(4-5) : shows density of state (DOS) and Energy (eV) of NiO as aferromagnetic and antiferromagnetic material at different values of magnetization ($0.2, 0.4, 0.6 \text{ A.m}^{-1}$).

From fig (4.2), fig (4.3), fig (4.4) and fig (4.5) , Show the differences of density of state (DOS) of NiO as ferromagnetic and antiferromagnetic behavior, And was found to be the density of state in ferromagnetic materials greater than antiferromagnetic, may be attributed to the Fermi energy (E_F) of NiO as ferromagnetic larger than antiferromagnetic and the magnetic moments of antiferromagnetic have opposite directions.



Fig(4-6) : shows band structure of NiO as antiferromagnetic and ferromagnetic material at different values of magnetization (0.2, 0.4, 0.6) $A.m^{-1}$.

From (4.6) explains there is no any relationship between band structure and magnetization for NiO as ferromagnetic and antiferromagnetic material.

4.2 Recommendations and Conclusion

In this study installation of quantum ESPRESSO and gnuplot. In quantum ESPRESSO the magnetic properties of NiO as ferromagnetic and antiferromagnetic materials are studied, band structures, density of state (DOS) are plotted using gnuplot, which shows the ferromagnetic behavior of NiO have high DOS than antiferromagnetic and have direct band gap.

4.3 References

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