STRUCTURAL AND ELECTRONIC PROPERTIES OF LITHIUM NITRIDE USING DENSITY FUNCTIONAL THEORY

kassa Adugna

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This is to certify that the thesis prepared by **kassa Adugna** Graduate Studies entitled " **structural and electronic properties of Lithium nitride Using Density Functional Theory**" in fulfillment of the requirements for the degree of **Master of Science** complies with the regulations of the University and meets the accepted standards with respect to originality and quality. .

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Supervisor: Dr. Menberu Mengesha

Readers: Dr. Nebiyu Gemechu

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Date: **March,24, 2023**

Author: **kassa Adugna**

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Signature of Author

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Abstract

In the calculation of structural and electronic property of lithium nitride (Li_3N) to investigate with density functional theory (DFT) using Quantum Espresso package. Our study is based on Density Functional Theory (DFT) with the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional, Vanderbilt (ultra soft) pseudopotentials and the plane wave basis set implemented in the Quantum-ESPRESSO package. The calculation of the total minimum energy and the total minimum force of Li_3N is calculated as a function of cutoff energy and K-points sampling. The total minimum energy per cell is monotonically decreasing with increasing cutoff energy due to variational principle. However, this trend can not be predicted from increasing the k-points sampling. Moreover, the equilibrium lattice constant is calculated using results obtained from energy convergence test (i.e., 80 Ry and -63.33138621. The computational value of the equilibrium lattice constant is 3.651 Å. This result is in good agreement with experimental value which is 3.501 Å . Finally, discussing band structure and density of state of two dimensional Li_3N, the electrical property of two dimensional Li_3N is determined based on energy band gap.

Keywords: Lithium Nitride, Density Functional Theory, Electronic and structural properties.

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Chapter 1

Background of the Study

1.1 Introduction

Lithium and nitrogen are two elements that are compound to form lithium nitride (Li_3N) and Lithium nitride's are mostly found the earth's crust, form naturally through the weathering Li-rock, in trace amount of soil and in the ocean. Lithium nitride is an inorganic compound with composed of Lithium (Li) and nitrogen (N). The number of electron configuration of a Lithium nitride respectively is $[He]2S^1$ or $1S^2 2S^1$ and nitrogen's are $[He]2S^2 2P^3$ or $1S^2 2S^2 2P^3$ .The molecular weight of Li_3N 36.8456g and the density of Li_3N is $1.3 g/cm^3$ and gravity 1.3 its melting point is $813c^o$ ($1495f^o$) and the color of solid Lithium nitride is reddish -pink and powder with high melting point[1]. Lithium is found in the rocks, soils and sea, and it's mineral forms, petalite and spodumens Lithium does not occur as native metal because it is so reactive and manufactured from chemical compound, there are large number of compound that contains Lithium some of which occurs naturally while the other are manufacturing in process of plant [2]. Lithium is a lightest metal, the least dense of all the element that are not gas at 20 percent and can float on water it is very soft, with hardness react easily with each and also not toxic it uses for treat some neurological disorder and to produce glass, ceramics, and reducing the points of compounds and batteries . Nitrogen can form compound with different element in the periodic table with chemical bonding ranging from covalent to ionic metal. Lithium nitride is only known thermodynamically stable alkali metal nitride, and it is ore of the most ionic of all known nitride,(3-5).

Lithium nitride used for two phase mixture $\alpha - Li_3N$ and $\beta - Li_3N$ can be prepared by direct combination of element ,Lithium with nitrogen gas at $400c^o$ [6].

The Crystal structure was evaluated first by Zint and Braur [7] and later in turn revised by Rabanau and Schulz[8]. They revised that the structure of $\alpha - phase$is hexagonal with $(p6/mmm)$ space group and lattice constant and $\alpha - Li_3N$ crystal structure consist of two types of layers in the lithium atom Li[1] are arranged in a graphite like structure with nitrogen atoms at the center of the hexagons in the pure lithium layer in the Li[2],are on the top of nitrogen atom $\alpha - Li_3N$ is known to have an exceptionally large Li ionic conductivity [9,10].

Its conductivity is caused by intrinsic defect [1-2]percent vaccines the $\alpha - Li_3N$ layer. Due to the defect within the layer ,the structure of $\alpha - Li_3N$ is packed loosely and consequently it could be expected of $\alpha - Li_3N$ [11] The $\alpha - Li_3N$ phase remain stable up to 35 GPa. The third solid phase of Li_3N is $\gamma - Li_3N$ exist at ultrahigh pressure, the theoretical calculation predicated the phase transformation from $\beta - Li_3N$ to a cubic structure p43mm at 37.9Gpa, [12] $\gamma - Li_3N$ furthermore experiment evidence showed that $\beta - Li_3N$ induced transforms to a cubic structure $\gamma - Li_3N$ is the pressure range of 36-45Gpa [13].Li_3N possess a FCC structure in the Fm3m space group and remains stable up to 200Gpa.

Lithium nitride is an important material which can be used for hydrogen storage due to its high theoretical H_2 capacity and also is component in the synthesis of nano phase GaN . Lithium nitride that can be used Co_2 conversion and electric charge storage and batteries. And compound with transition metal (M),Li_3M_xN are excellent ionic conductor .[14,15]

Density functional theory [DFT] is the most important quantum mechanical approach to study matter.

It is now days applied for computations of ground states properties of molecules and solid , the binding energy of molecules and the band structure of solid in physics and for calculation of the bulk ground state properties for a lattice constant, bulk modulus, cohesive energy and atomic position s play an important role in the physics of condensed matter [16].

Ab-intio calculation were employed to evaluate the band structure of Li_3N, Kerker,s self-consistent electronic structure calculation for $\alpha - Li_3N$ predicted that the energy gap between the occupied valence band and the lowest excited band 1ev[17] and carried out density functional calculation with plane wave pseudo potential method, predicting that the energy gap of $\alpha - Li_3N$ at pressure of 0,GPa.[18].

The electronic property were computed on $\alpha - Li_3N$ using density functional theory[DFT] to compare the behavior of a monolayer of Lithium nitride with respect to the bulk material and to develop an understanding of the evalution of electronic structure Li_3N with the number of layer as compared to graphene and other van-der Waals nano structure [VdWNS] our calculation confirm that bulk, $\alpha - Li_3N$ is semiconductor with an indirect band gap of in agreement with several previous first principle calculation of the $\alpha - Li_3N$ electronic property .[19,20]

Effects of interactions and correlation of electron structure and other finite systems. The remarkable successes of the approximation local density[LDA] and generalized -gradient approximation [GGA],functional within the Kohn-sham approach have let to widespread interest in density functional theory as the most promising approach for accurate practical method in the theory of materials. Help us to understand character and predicate mechanical properties of materials in surrounding, under extreme condition. The aim of this research is to study structure and electronic properties of Lithium nitride based on density functional theory using quantum espresso package.

1.2 Statement of the problem

It is known that the Schrdinger equation of many body problems are difficult to solve analytically, Li3N is a system with many electron, current year, there will be a remarkable approach to solve such compound using density functional theory numerically, the fundamental tenet density functional theory is that any property of the system of many interacting electrons can be viewed as a functional of the ground state density $n_o[r]$;This functional is then in principle determines all information in the many body wave functions for the states. Therefore the purpose of this study is to investigate the structural and electronic properties of Lithium nitride using DFT[21]

1.3 Basic Research Question

- What is the total minimum energy of Lithium nitride per cell with respect to cut-off energy?
- What is the total minimum energy of Lithium nitride per cell with respect to K point sampling?
- What is the total minimum force of Lithium nitride per cell with respect to cut-off energy?
- What is the total minimum force of Lithium nitride per cell with respect to K-point sampling?
- What is the value of lattice constant of Lithium nitride with respect to cut- off energy ?
- What is the band structure of Lithium nitride?
- What is the density state of Lithium nitride?

1.4 Objective

1.4.1 General Objective

The general objective of this study is to calculate the structural and electronic properties of lithium nitride with respect to density functional theory.

1.4.2 Specific Objectives

Specific objective of this study are:

- To calculate the total minimum energy of Lithium nitride per cell with respect to cut-off energy?
- To calculate the total minimum energy of Lithium nitride per cell with respect to K-point sampling?
- To calculate the total minimum force of Lithium nitride per cell with respect to cut -off energy ?
- To calculate the total minimum force of Lithium nitride per cell with respect to K-point sampling?
- To calculate the lattice constant of Lithium nitride per cell with respect to cut-off energy?
- To calculate the band structure of Lithium nitride using DFT?
- To calculate the density of stated [DOS] of Lithium nitride? using DFT?

1.5 Significance of the study

The importance of this study is to understand the structure and electronic properties of Lithium nitride [many electron system] using new computational technique

.And also helping to know the exact value of lattice constant of Lithium nitride of conductor of a crystal in a solid material will allows scientists to know many of the properties of Lithium nitride under different conditions. Moreover, it is important to understand, the electrical property of three dimensional Lithium nitride and help to compare the experimental results with respect to calculation.

1.6 Scope of the study

The scope of this study will limited to calculate the total minimum energy of Lithium nitride and minimum force of Lithium nitride with lattice constant of Lithium nitride using cut-off and K -point

.

Chapter 2

Review of Related Literatures

2.1 Introduction

This chapter begins explanations with basic concepts of density functional theory Schrdinger Equation and approximations made on it area then explained, Next , Hohenberg-Kohn theorem, which are the central part of density functional theory and Kohn-Sham equations are presented briefly. Exchange-correlation energy functional and approximations (such as local density approximation and general gradient approximation) which make Kohn-Sham equation easier are also being presented. Finally pseudo-potential, energy cut-offs, K-point samplings are explained in detail.

2.2 Densityfunctional theory [DFT]

Density functional theory [DFT] is the most popular and versatile method in condensed matter physics or computational physics as well as computational chemistry .It is a quantum mechanical method that is widely used to investigate the electronic structure of many body system particularly molecules and condensed phases.[22] Density functional theory is also successful quantum mechanical molecules, clusters homogenous solids surface and interfaces, quantum wells ,quantum dots and other [23].It is now a days used for calculating, The binding energy of molecules in chemistry and the band structure of solid in physics. First application relevant for fields tradition only considered more distance from quantum mechanics, such as biology and mineralogy are begging to appear ,superconductivity atoms in the focus of strong laser pulses ,relativistic effects in heavy elements and in atomic ,classical liquid ,and magnetic properties of alloys have been study with DFT is neither, HF method not post-HF method .The wave functions for spin and spatial parts are constructed in a deferent way from those in HF and the induced orbital's are often referred to as Kohn-sham' orbital Nonetheless, the same procedure of SCF is used as in HF theory function with electronic density as the basic quantity . The main objective of density functional theory is to replace the many body electronic wave function with the electronic density as the basic quantity.

2.3 Schrodinger's Equation

Any problem in the electronic structure of matter is covered by Schrodinger equation including the time .In most cases however, One is concerned with atoms and molecules without -time dependent interaction, so we may focus on the time-independent Schrodinger equation .The stationary Schrodinger equation [24]is calculates as

$$H\Psi_i[X1, X2...XN, R1, R2...RM] = E_i\Psi_i[X1, X2...XN, R1, R2...RM] \qquad (2.3.1)$$

Where H is the Hamiltonian for a system consisting of M nuclei and N electrons and E the total energy of the system .The solution to this equation gives us the total wave function ω which is in principle contains all wanted properties of the system and is therefore essential in quantum mechanics. The goal is to find this wave function equivalently, as in the case of density functional theory.

$$n[r] = |\Psi|^2 \qquad (2.3.2)$$

The density for the many body problems of a system containing N electron and K nuclei with charge Zi the Hamiltonian calculated as(25)

$$\hat{H} = \frac{-1}{2}\sum_{i=1}^{N}\nabla_i^2 \frac{-1}{2}\sum_{A=1}^{m}\frac{1}{M_A}\nabla_A^2 - \sum_{i=1}^{N}\sum_{A=1}^{N}\frac{ZA}{riA} + \sum_{i=1}^{N}\sum_{j=i}^{M}\frac{1}{rij} + \sum_{A=1}^{M}\sum_{B>A}^{M}\frac{ZAZB}{RAB} \quad (2.3.3)$$

The first two term s represent the kinetic energy of the electron and nucleus.T_e and T_n. The third term represents the electrostatics repulsion between the electron.Vee. The fourth term represents the electrostatics between the electrons and nuclei .Vne, and the last term between the nuclei, V_{nn}, is the mass of the electron Me and mass of the cores is Mz .ZA is the number of protons in each core. This looks rather complicated.It turns out that the stationary Schrodinger equation can only be solved analytically for one electron system e.g the hydrogen atom or the ionized helium atom He+,so to be able to continue, certain approximations have to be made.

2.4 Born-Oppenheimer Approximation

As a first approximation one usually makes the Born-Oppenheim approximation[26] which is justices by the fact that the nuclei(ions) are much heavier than the electrons Mji¿¿ me in most cases, this justices a time-scale separation by saying that the electron immediately adapt to changes in the positions of the ions. This means that the electronic and system can be treated separately and for the electrons the ions can be regarded as fixed. We can therefore drop the ionic kinetic energy term and the ion-ion interaction term in the Hamiltonian and only consider the terms involving Born-oppenheimer approximation due to their masses the nuclei more much slower than the electron. We can consider the electrons as moving in the field of fixed nuclei, the nuclear energy is zero and their potential energy in merely a constant. Thus, the electronic Hamiltonian reduce to

$$\hat{H_{ele}} = \frac{-1}{2}\sum_{i=1}^{N}\nabla_i^2 - \sum_{i=1}^{N}\sum_{A=1}^{M}\frac{ZA}{riA} + \sum_{j=i}^{N}\frac{1}{rij} = T_e + V_{ne} + V_{ee} \quad (2.4.1)$$

The solution of Schrodinger equation with H_{ele} is the electronic wave function $\Psi_{electro}$ orΨ_{elec}, and the electronic energy E_{ele}.The total energy E_{tot} then the sum of E_{ele},and the constant repulsion E_{nuc}.

$$H_{ele}\Psi_{ele} = E_{ele}\Psi_{ele} \tag{2.4.2}$$

$$H_{tot} = E_{ele} + E_{nuc} Where E_{nuc} = \sum\sum \frac{ZAZA}{RAB} \tag{2.4.3}$$

2.5 The Hohenberg-Kohn Theory

Hohenbeng-kohn is to formulate density functional theory as an exact theory of many body Type equation here.systems. The formulations apply to any system of interacting particles. The Hk formalism [27] Of DFT is based on two theorem.

2.5.1 Theorem I

The external potential is a unique functional of the electron density$n_o(r)$ only thus, the Hamiltonian and hence all the ground state properties are determined solely by the electron density. This theorem implies that the Hamiltonian, H, determines the ground state of the system. All the other interaction potentials and the kinetic energy will be a functional of$n_o(r)$.

2.5.2 Theorem II

Thesecond HK theorem define energy density functional for the system and proves that the correct ground state electron density minimize the energy functional [28] .The energy functional of the density $f_n$is

$$E(n) = \int drVex(r)(n) + F(n) \tag{2.5.1}$$

Where F(n) is universal functional of the density and incorporates the kinetic and the potential energy .Once the external potentialVex_r has been fixed ,the energy functionalE_n has its minimum the ground state energyE_o, at the physical ground states density $n_o(r)$

$$E(o) = E(n] \tag{2.5.2}$$

The Hohenberg-kohn HK) theorem have the limited purpose to prove that a universal functional of the electron density exists; they do not derives its actual expression for the kinetic energy as a functional of n is known except for simple metals. The Kohn-sham(ks) scheme are formulation of the theory based on the ks orbital's instead of the more density ,is the starting -point of most of actual calculation term E_{xc}, whose exact from is not known to make the formalism useful, it is necessary to make some approximations for the exchange correlation term $E_{xc}(n)$.The most common and straight forward approximation to$E_{xc}(n)$ is the local density approximation(LDA) [29]. The idea of the LDA is assuming that the exchange -correlation energy per electron of a non -uniform system at any point in space is equal to the exchange-correlation energy per electron in a uniform electron gas having the same density at this point ,in LDA the exchange-correlation functional can be write as

$$E_{xc}^{LDR}[n] = \int drExc[n]n[r] \tag{2.5.3}$$

$$Exc[n] = Exc[r] \tag{2.5.4}$$

By definition , the LDA is local because the exchange -correlation energy E_{xc} (n) each point in space only depends on the electron density at the same point. The $E_{xc}(n)$ has been calculated and parameterized through Monte Carlo total energy calculation for a uniform electron gas with a Varity of electron density [30]. Since the LDA is based on uniform electron gas, it is expected to be accurate only for systems in which the electron density varies slowly, it is clearly not suitable for the situations where the electron density undergoes rapid changes, as in the covalent bounded solids. To overcome this deficiency of the LDA, another from of exchanged -correlation functional will be developed, that is the generalized gradient approximation(GGA) [31].

2.6 Kohn-Sham Equation

The density functional theory[DFT],in the kohn-sham formalism , provides a powerful computational scheme, which allows determining exactly the ground state properties even if complex systems of interacting particles, simply solving a single particle like equation ,kohn-sham density [32] is widely used for self-electronic structure calculations of the ground state properties of atoms ,molecules and solids, The Kohn -Sham equation.

$$HKS\Psi_i = [\frac{1}{2}\nabla^2 i + Vex(r)]\psi_i = E_i\psi_i \tag{2.6.1}$$

whereVex_r external potential Ψ_i Eigen function within frame work of Kohn-sham DFT(ksDFT) the intractable many-body problem of interacting electron s in a static external potential reduced moving to a tractable problem of non-interacting electrons moving in an effective potential .The effective potential includes the external potential and the effects of the coulomb interactions between the electrons e.g the exchange and correlation interactions, modeling the latter two interactions becomes the difficulty within ks DFT[33].

2.7 Exchange-Correlation Energy

The ks DFT provide a practical procedure to solve the many-body problem by breaking the problem in to a selecting particle problems .This formation is exact but practically still un soluble since the many-body wave function are still included in the exchange-correlation. The GGA functional depends on the local electron density as well as the spatial variation of the electron density that is represented by the density gradient. The GGA functional can be written as

$$E_x c^{GGA}(n) = \int dr Exc(n) E[nn] n(r) \tag{2.7.1}$$

$E_{xc}(n)$ is the exchange correlation energy per particles of an electron gas and F_{xc} is functional of the electron density and its gradient .The GGA method gives better total energy especially for small consuming than LDA [34].Generally GGA has the following advantage over LDA [35]. GGA improves ground state properties for light atoms, molecules and cluster. GGA predicts the correct magnetic properties of 3d metal such as body centered Lithium. Through GGA seems to be superior compared to LDA .It has several draw backs. A GGA method fails to accurately treat the hydrogen bond. This defect is clearly manifested through expansions and hence softening of bonds [36].

2.8 Periodic Boundary Condition K-Point Sampling

each electron, the electronic wave function extends in the entire lattice, and thus the basis set required to expand the ks orbital's is infinite too. Fortunately, perfect crystallized solids can be described as spatially rapidly repeated unit cells that only contains a small number of electron and nuclei, This leads to the uses of periodic boundary condition through the Bloch theorem ,which confines the study of a very large number of electron in to a single unit cell.

2.9 Blochs Theorem

Blochs theorem states that in a periodic solid each electronic wave function can be written as the product of cell-periodic part and wave like part[39].

$$\Psi_k(r) = e^{ik.r}U_K(r) \tag{2.9.1}$$

where uk(r) is periodic in space with the same periodicity as the supercell.That is,$uk(r + n_1a_1 + n_2a_2 + n_3a_3)$ uk(r) for any integers n1, n2, and n3. This theorem means that it is possible to try and solve the Schrodinger equation for each value of wave vector k independently. The cell-periodic part of the wave function can be expanded using a basis set consisting of a discrete et of plane waves whose wave vectors are reciprocal lattice vectors of the crystal

$$U_K(r) = \sum_G C_iGe^{iG.r} \tag{2.9.2}$$

Where the recporical lattice vectors G are defined by $G.l = 2\pi(n)$ all there is a lattice vector of the crystal and n is an integer. Therefore each electronic wave function can be written as a sum of plane waves

$$\Psi_r = \sum_G C_{ik} + Ge_{i(K+G).r} \tag{2.9.3}$$

The electronic wave functions at each k.point are now expressed in terms of a discrete plane wave basis set. In principle this Fourier series is infinite. However, in practice we cannot work with an infinite basis set, it has to be truncated. The number of plane waves can be restricted by placing an upper boundary to the kinetic energy of the plane waves. This boundary is called energy cut-off Ecut. The Bloch theorem state that the solution of the single particle Schrodinger equation (i.eks equation) in the presence of proposal form.

$$\Psi_i(kr) = e^{ikr}u_i(kr) \tag{2.9.4}$$

Where ui (k.r) is the cell-periodic part of the wave function such that$ui(k.r)$=$Ui(k.r+R)$ for all lattice vectors R, The variable R is the wave vector of the first Brillion zone (BZ) Thus

$$\Psi_i(kr + R) = \Psi e^{ikr} \tag{2.9.5}$$

substituting Eq [2.6.5] in to ks equation Eq[2.5.1] a new equation is found each for a given k each electron occupies an electronic state of define wave vector k .Therefore, the problem of solving for an infinite number (103) of electrons within the extended system is converted to solving for a finite number of electronic bands at an infinite number of k-point within the single(reciprocal) unit cell, changing from one infinite number to another however, does not directly make the problem simpler. Nevertheless , the electronic wave function at the k-point that are very close to each other will be almost identical, and therefore in practice one can represent the wave functions over a small region of reciprocal space around one k-point by the wave function at this k-point .In this case ,only a finite number of k-point are needed to determined the ground state of solids .The density of allowed k -points is proportional to the volume of the solid [37] many efficient schemes have been developed for the k-point sampling in the first BZ using these schemes , one can obtain very good approximation for the electron potential and total energy of solid .The idea is to represent any integral over almost continuous k-points in the first BZ by the summation over a k-point sampling

$$\frac{n}{2n_3}\int dr \tag{2.9.6}$$

$$f(k)=\sum_i f(k)\Psi_i \tag{2.9.7}$$

was developed Type equation here. by monk horst and park [38] the so called MP meshi. The MP mesh utilizes the space group symmetries of the lattice and cretins the sampling only in the irreducible wedge of the first BZ. The k-point are also selected according to their point groups symmetries , which in turn decides the weight .In this way, a sufficient sampling can be achieved in a very small number of k-point .The magnitude of error in the calculation total energy due to insufficient k-point sampling can always be reduced by using a denser k-point mesh ,with sufficient k-point, the computed total energy will converge and the error due to the k-point sampling approach zero.

2.10 The Plane Wave Basis Set

With the approximation of exchange -correlation term and using the periodic boundary condition it is possible to solve the ks boundary equation Eq [2.5.1] in order to solve the ks equation numerically, the ks orbital's need to be expands by some well-defined basis sets. Although there are many chooses of basis sets a variable [39] the plane wave (Pw) basis sets is probably the most straight forward. The plane wave are not centered at atoms, moreover it form a compete basis set with very simply mathematical functions. The completeness of the basis set is easy to adjust ,essentially through only one parameter ,i.e kinetic energy cut offE_{cut}. The ks orbital's $\Psi_i(k.r)$ can be

$$\Psi_i(Kr) = e^{u_i(kr)}\frac{1}{\sqrt{v}}\sum_{ci} k + re^{i(kr)} \tag{2.10.1}$$

Where G is reciprocal lattice vector is the crystal volume and ci are coefficient in the expansion. In principle, an infinite basis set of G Should be used to expand the ks orbital's Ui(k.r).In principle ,it is possible to truncate the infinite basis set to include only Pw's that have kinetic energy less than a defined cut off energy.

$$\frac{\hbar^2 2m}{|k^2 + G^2|} \leq E_{cut} \tag{2.10.2}$$

Where Ecut is called the kinetic cut off . Pw's have many attractive features ; they are simple orthogonal by construction, unbiased and it very simply to check for convergence by increasing the cut off.

2.11 Pseudo potential

The Phillips-Kleinman Construction The pseudo potential approach originated with the orthogonalized plane wave (OPW) method [32], in which the valence wave functions were expanded using a basis consisting of plane waves that were orthogonalized to the lower lying core states,ψ_i

$$\Phi(opw)(K+G) = \phi(opw)(K+G) - \sum_{\alpha c} < \varphi_c|\varphi(pw)(K+G) > \varphi_{\alpha c} \tag{2.11.1}$$

where ϕ^{PW} is a plane wave and ϕ^{OPW} is the corresponding OPW, and the sum is over core states and atoms. Pseudo-potentials were introduced to model the interaction between ions and valence electrons. They effectively eliminate, from the very start, the true electron nuclear potential and the inner core electrons, that is, those electronic states which are tightly bound to the nucleus, do not participate in the formation of chemical bonds, and remain approximately unchanged in atoms, molecules, and solids [33,34]. This tremendous conceptual simplification also amounts to a very practical and efficient computational scheme, especially when a plane-wave basis set is adopted to expand the electronic wave functions. After1980,this method, in connection with a density-functional description of the electron-electron interaction, evolved into a reliable prescription for the first-principles computation of electronic, structural, and dynamical properties of molecules and solids. The fundamental idea of pseudo potential is the replacement of one problem with another. The primary applications in electronic structure is to replace the strong Coulomb potential of the nucleus and the effects of the tightly bound core levels by an effective ionic potential acting on the valence electrons. The corestatesremain almost unchanged (Frozen approximation). Plane wave pseudo potentials are usually employed because of the extreme simplicity. The strong core potential is replaced by a pseudo potential. For many elements the resulting pseudo wave functions are quite smooth.

2.12 Model Ion Potential

Pseudo potential has become a fertile field for generating new methods and insight for the electronic structure of molecules and solids. There are two approaches:- Ionic Pseudo potential, i.e., for better transferablity and total pseudo potential for describing bands accurately. Pseudo potential has the following goals:

(1) Pseudo potential should be as soft as possible, meaning that it should allow expansion of the valence pseudo-wave equations using as few plane waves as possible.

(2) It should be as transferable as possible (meaning that a pseudo potential generated for a given atomic configuration should reproduce others accurately).

(3) The pseudo-charge density (the charge density constructed using the density-wave functions) should reproduce the valence charge density as accurately as possible [39,40,41]

2.13 Norm-Conserving Pseudo potential

The pseudo-wave function (and potential) are constructed to be equal to the actual valence wave function (and potential) outside some core wave function radius r_c. Inside r_c, the pseudo-wave functions differ from the true wave function, but the norm is constructed to be the same. The integrated charge density inside $r_c$for each wave function agrees. The wave function and eigenvalue depend on the angular momentum L. The pseudo wave function should be L dependent and is called semi-local.

In position of norm conservation ensures that the logarithm derivative (scattering property) of pseudo and all electron wave functions much of reference energy [E] and the first derivative with respect to E matches as well. Norm conserving pseudo potential has a special class in the development of ab initio pseudo potential and generated by calculations on atoms and cant be fitted to experiment.

2.14 Ultra Soft Pseudo potential

Ultra soft pseudo potential defines an auxilary function added to the plane waves around each atom and allows fewer plane waves for good description. This is in sprit of OPW but with smooth auxilary function. Vanderbilt and co-workers [35-37] proposed a radical departure from the concept of norm-conservation. In their approach, the pseudo-wave functions are required to be equal to the all-electron wave functions outside r_c, as with norm-conserving , but inside r_c they are allowed to be as soft as possible; the norm-conservation constraint is removed to accomplish this. Although this introduces some complications, it can greatly reduce the plane wave cutoff needed in calculations, particularly since quite large values of r_c can be used in their scheme The complications that result are two-fold. First of all, since the pseudo-wave functions are equal to the all electron wave functions (and therefore have the same norm) in the interstitial, but do not have the same norm inside r_c they are necessarily not normalized. This introduces a non-trivial overlap into the secular equation. In fact, the overlap turns out to be non-diagonal. Secondly, the pseudo charge density is not obtained by computing P ?*? as with norm conserving ; among other things this would yield the wrong total charge. Rather, an augmentation term needs to be added in the core region. A third, but less important, complication is that by relaxing the norm conservation, the resulting pseudo potentials can become less transferable. However, Vanderbilt pseudo potentials were proposed for use in large scale calculations, for22 which the cost of generating pseudo potentials is negligible compared with the cost of the calculations. Accordingly, it is quite feasible to recalculate the pseudo potential as the configuration evolves during the course of the calculation [38].

2.15 Periodic Super cells

In solid-state physics , a crystal structure is described by a unit cell. There are an infinite number of unit cells with different shapes and sizes which can describe the same crystal by lattice vectors a_1, a_2, and a_3. If we solve the Schrodinger equation for this periodic system, the solution must satisfy a fundamental property known as Blochs theorem.

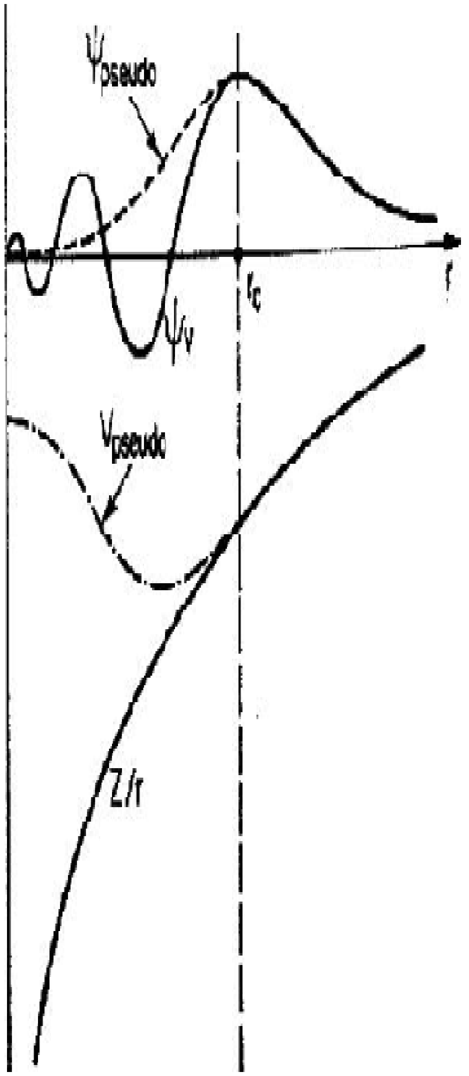

Figure 2.1: *function and core potential by a pseudo-wave function and psuedopotential.*

Chapter 3

Research Methodology

3.1 Materials and Method

3.2 Materials

The study is purely theoretical .The main source of information are the published articles books ,thesis and dissertation ; soft ware's and computers are additional instruments used to accomplish this project.

3.3 Computational Methodology

The electronic structures of lithium nitride is obtained by kohn-sham density functional theory[40].using Quantum Espresso package [41 -42] quantum ESPRESSO is an integrated suite of computer codes for electronic -structure calculation and material modeling based on density -function theory(DFT) [43].plane wave basis sets (PW) and pseudo potential [44].It is freely available and additional as open-source soft wave under the term of the GNU General public license. In the approximation of the potential, the core electrons which do not participate in the chemical bonding of the system are frozen and only valence electrons are considered. For convergence tests, the electronic wave functions are expanded in a plane-wave basis set with trial cutoff energy. The k-point sampling of the Brillouin zone was constructed using Monk horst and Pack mesh scheme [47]. Convergence test of total energy with respect to energy cutoff and k-point sampling is performed to ensure the accuracy of the calculations until the change in energy is equal to 0.01 eV. The computation is taken place in such a way that input file is given for the software(quantum ESPRESSO Package). The input file is composed of three name lists, control and system, electrons, followed by three cards ATOMIC SPECIES, ATOMIC POSITIONS, K-POINTS. During computation the system follows Algorithm of Self-Consistent Iteration. Self-consistent iterations to solve this problem consist of starting with an initial guess of the charge density n(r), then obtaining a guess for Vext and solving Kohn-Sham equation for wave function $\Psi_i(r)$ to update charge density and external potential. Then, Kohn-Sham equation is solved again for the new wave function and the process is carried on until the difference between two consecutive external potential is below a certain tolerance (equivalently, the wave functions are close to stationary)[48]. The SCF method is an iterative procedure which yields a self-consistent set of wave functions and orbital energies. Flow chart scheme of SCF to iterate Kohn-Sham equations for a set of fixed nuclear (ionic) positions is shown in the figure below

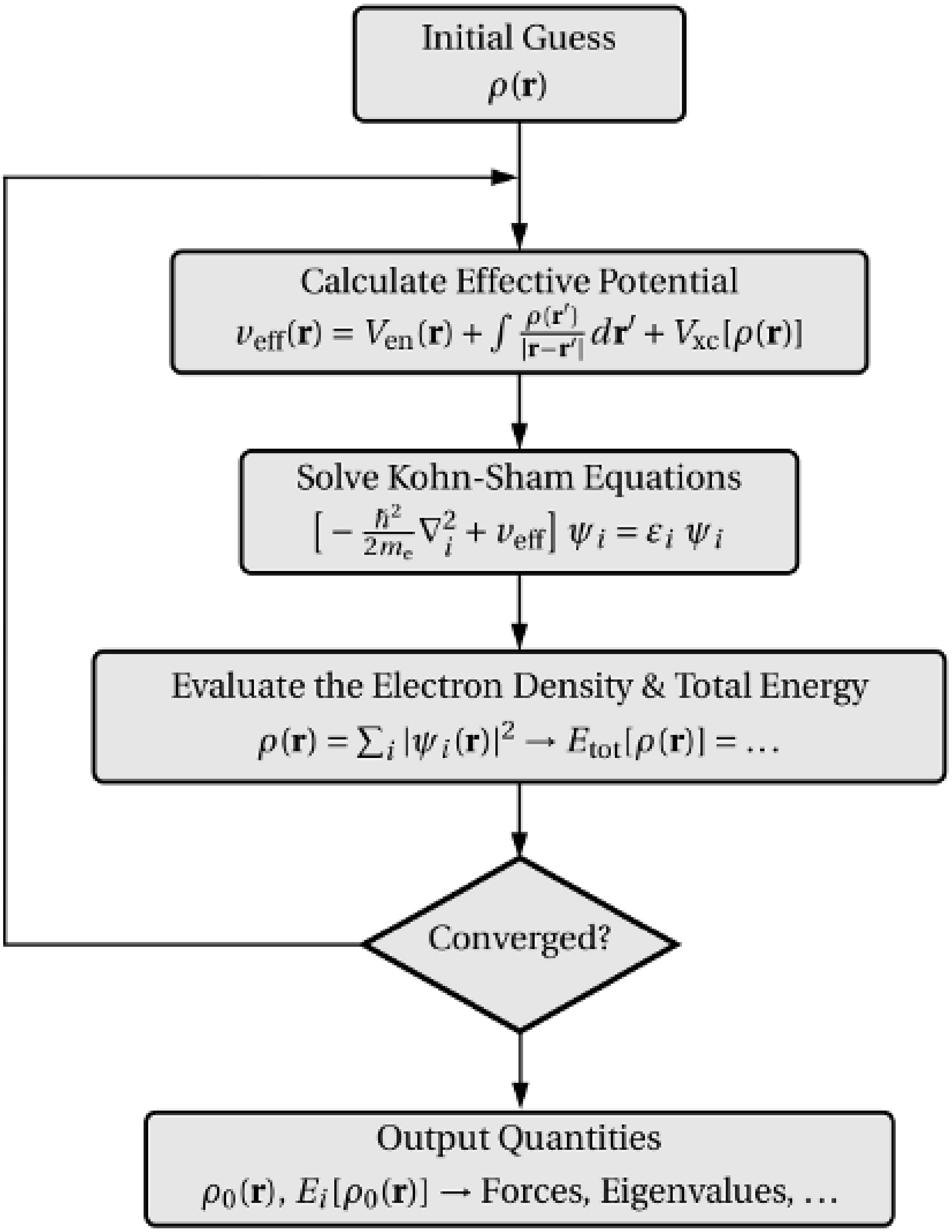

Figure 3.1: *Self Consistent Field of flow chart of the iteration scheme.*

Chapter 4

Results and Discussions

4.1 Introduction

In this chapter, the structural and electronic properties of Lithium nitride Li_3N, is calculated within the frame work of the density functional theory. The important aspects in studied Lithium nitride are the total minimum energy and total minimum force, lattice constant, band structure and density of state of Li_3N. Results are mainly presented in figures. The first results are the total minimum energy per cell with respect to cutoff as well as K-points sampling and second results are total minimum forces values for there dimensional $Li3N$ with respect to energy cutoff and K-points sampling. Then comes the results for the equilibrium lattice constants, band structure and density of state of Li_3N. All results are presented in figures.

4.2 Geometrical Structure of hexagonal Li_3N

Li_3N has hexagonal structure with eperimental lattice constant a=3.651A^0 and c=3.889A^0 . The layer of [Li-N-Li-Li] structure

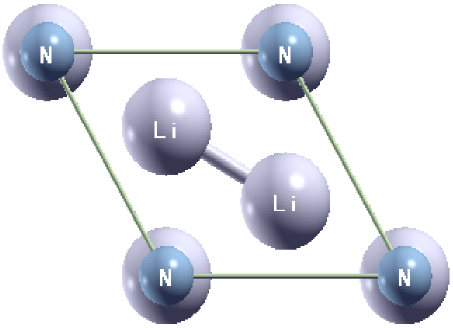

Figure 4.1: *Geometrical Structure of* Li_3N

4.3 Convergence Test of Total Minimum Energy of Li_3N with respect to energy Cutoff

The total minimum energy of Li_3N is calculated as a function of energy cutoff. In this case the input code has $3 \times 3 \times 3 = 27$ K-points mesh and lattice constant of 3.651 A. The calculation was done using different cutoff values, from 20 to 200 Ry. An increment of energy cutoff for wave function is made until the convergence is achieved (i.e the place where the energy becomes nearly constant). The total minimum energy converges at 80 Ry plane wave cutoff energy and the total ground state energy had its minimum at -63.37054774 Ry. Moreover, the total minimum energy is decreasing with increasing energy cutoffs for wave function. The accuracy of the ground state energy depends on the number of basis functions. However, we can get energy that close to ground state energy as the number of basis functions approaches infinity. As we can see from the Figure 4.2

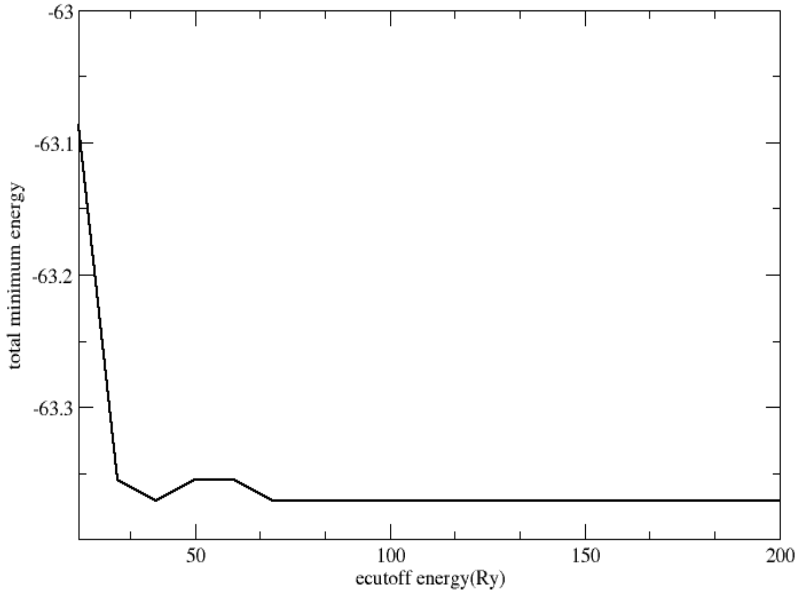

Figure 4.2: *Total minimum energy of* Li_3N *with respect to energy cutoff*

4.4 Convergence Test of Total Energy of Li_3N with Respect to K-point grid

In this case, the calculation was done using different k-point values from $2 \times 2 \times 2$ to $20 \times 20 \times 20$ k-points. The other variables such as lattice constant, energy cutoff, are kept fixed. The total minimum energy of Li_3N is calculated as a function of k-points grid size using PWSCF code. The total energy of Li_3N versus k-points grid size is shown in Figure 4.3. It can be observed that the total minimum energy of Li_3N converged at $8 \times 8 \times 8$ K-points grid and the total ground state energy has its minimum at -63.08716037 Ry.Figure 4.3

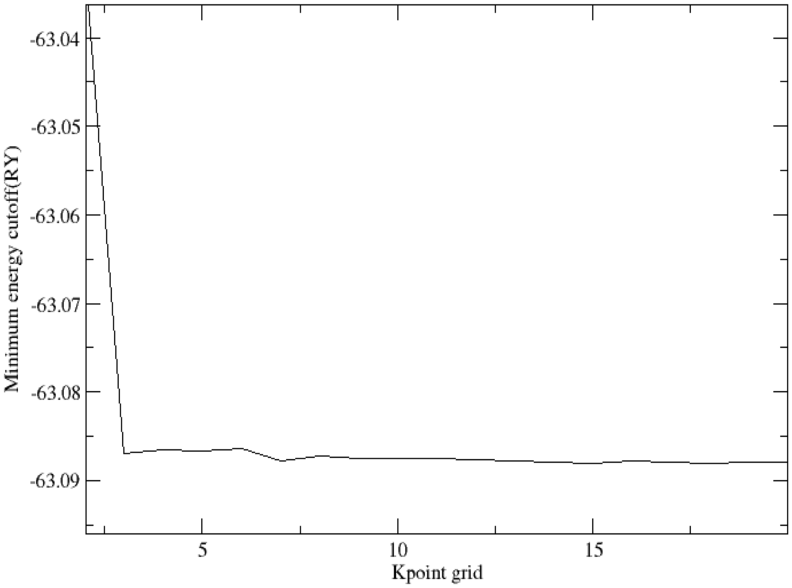

Figure 4.3: *Total minimum energy of Li_3N with respect to k point sampling*

4.5 Convergence Test of Total Force of Li_3N with Respect to energy Cutoff

Initially the net force acting on Li_3N in x,y and z directions is zero as a result of symmetry. However,when a Li atom was displaced by +0.05 in the z directions,net force is created The in put file is then set at value of lattice constants a= 3.651 c= 3.889 and k.points grids $2 \times 2 \times 2$. Finally,calculation was taken place at each value energy cutoff ranging from 20 Ry to 210 Ry with 10Ry intervals.The graph energy cutoff against total force acting on Li_3N The graph shows convergence is achieved at energy cutoff 80 Ry corresponding to minimum force on Li_3N is 286.302306 Ry and shwon in the Figure 4.4

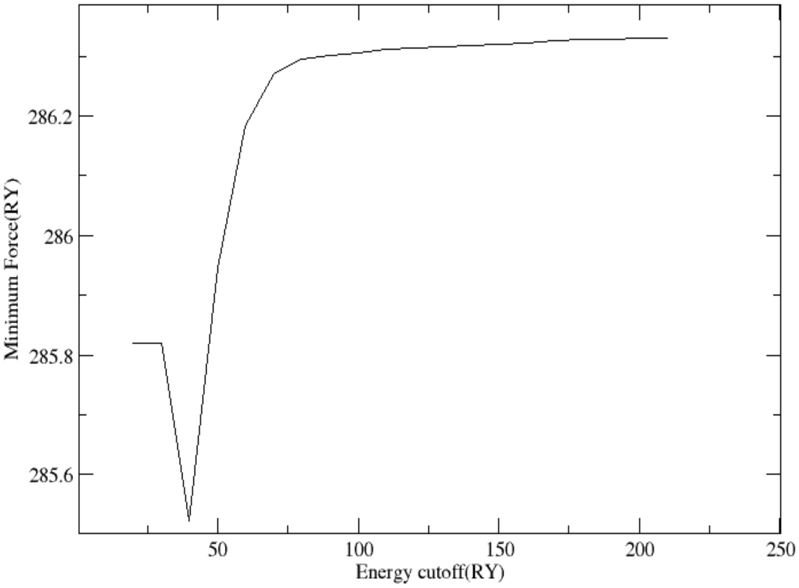

Figure 4.4: *Total force of Li_3N with respect to energy cutoff*

4.6 Convergence Test of Total Force of Li_3N with Respect to K-point grid

In this case, the calculation was done using different k-points value from $3 \times 3 \times 3$ to $19 \times 19 \times 19$. Here the other variables such as lattice constant, energy cutoff are kept fixed. As it is observed in Figure, the total force converges at the grid size of $8 \times 8 \times 8$ k-point mesh; and its value is 285.518053 Ry AA. Generally, it is true that different structural geometries will require different k-point meshes in order to reach convergence.

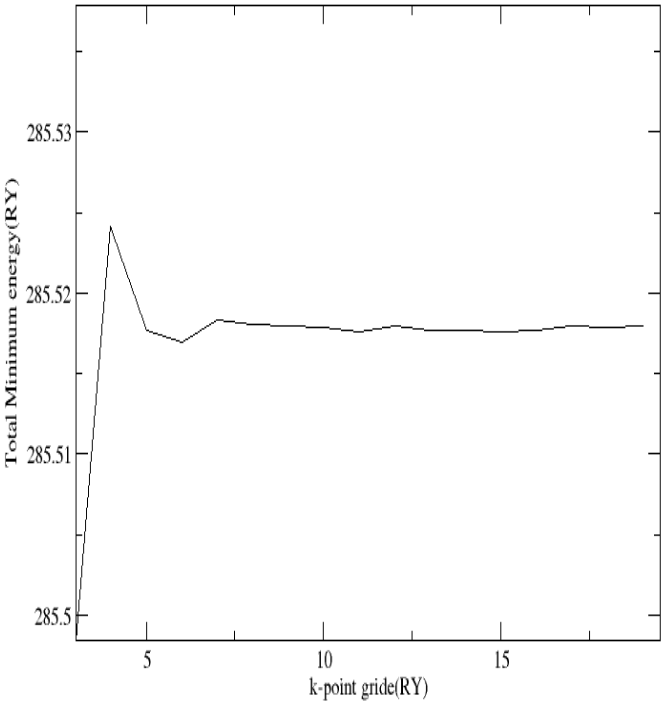

Figure 4.5: *Total minimum force of Li_3N with respect to k-point sampling*

To find the theoretical equilibrium lattice constant of Li_3N we varied a lattice parameters from 2.551to 4.401 In this calculation the minimum force and the K-points sampling are made fixed.And the interval =0.15, 80 Ry,-63.33138621(RY) The numerical calculation shows that the equilibrium lattice constant is 3.501 A. This result is in good agreement with experimental value.Figure 4.6

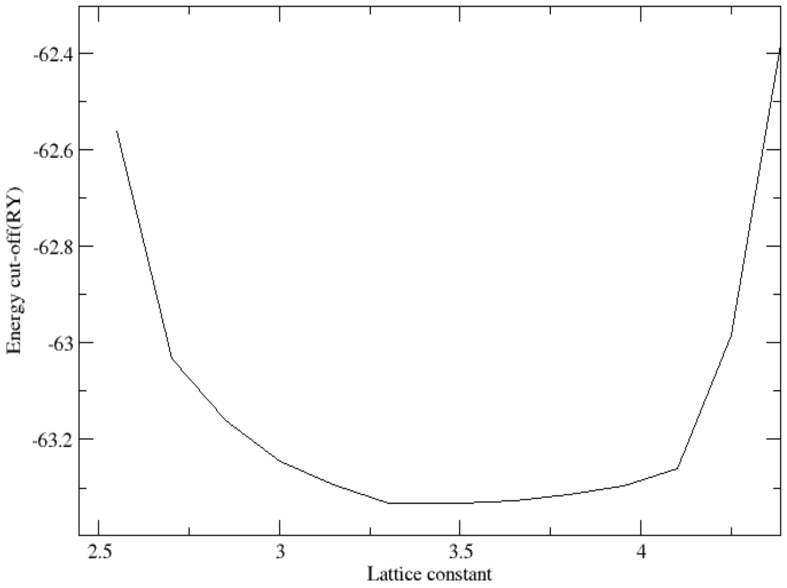

Figure 4.6: *Total energy of Li_3N versus lattice constant*

4.7 Band Structure of Two Dimensional Li_3N

In this work, the energy cutoff and the BZ sampling were chosen to converge the total energy with a value of 20 Ry and we generated 32 K-points in crystal coordinate. The energy band structure of the Li_3N is presented in Figure 4.7. Energy gap between occupied and unoccupied energy levels is among the ways that we can determine the difference between electrical properties of metals, semiconductor, and insulator. From band structure of Li_3N , we calculated the energy gap which is 1.1 eV. The calculated value has 0.082 percent of error with experimental value (2 eV). Li_3N is an indirect gap semiconductor material.we notice that there exist a double degenerate band in the Gama.A path just below the level as shwon in figure 4.7.This double degenerate

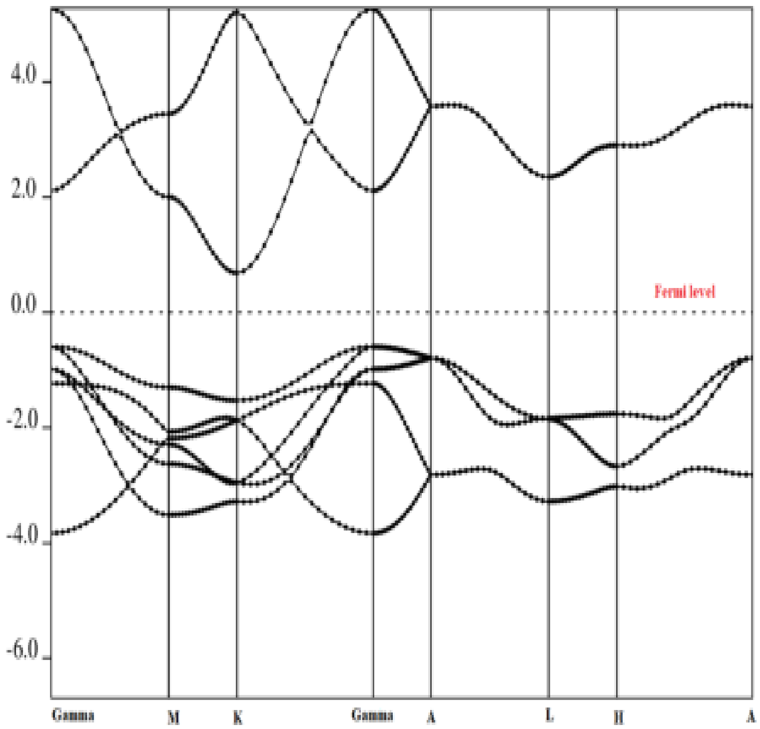

Figure 4.7: *Band Structure of mono-layer 2D* Li_3N

nodal line can be seen as nodal line.

4.8 Density of State (DOS) of Li_3N

The main issue we can see from calculating the DOS of Li_3N is the investigation of electronic transport properties of Li_3N. From the following Figure 4.8, we see that before the Fermi level enters the conduction band, there is an insulating regime. The Fermi level was referenced at 0 eV. The calculated energy gap of single-layer of Li_3N between the occupied and unoccupied energy levels was 1.1 eV and has 0.082 percent of error with experimental value. Semiconductor materials are a sub-class of material distinguished by the existence of a range of disallowed energies between the energies of the occupied level (valence electrons) and the energies of unoccupied level. Intrinsic semiconductors has band gap between 1 eV and 3 eV. Since so, our calculated value shows as our system is semiconductor.Figure 4.8

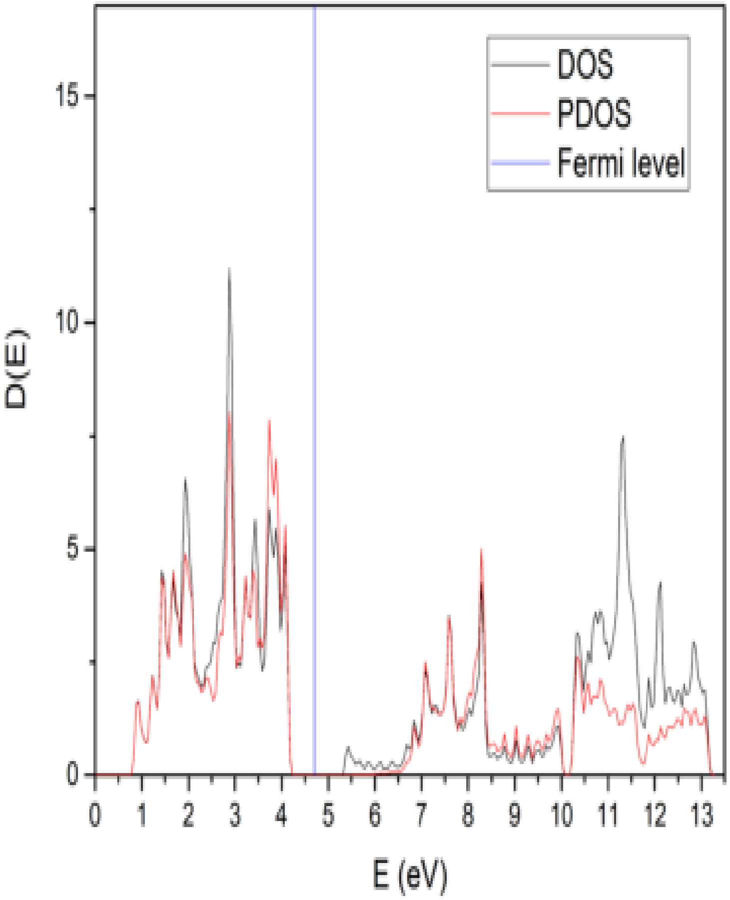

Figure 4.8: *Density of state of Li3N*

Chapter 5

Conclusion

In this thesis, we investigated structural and electronic properties of two dimensional Li_3N using DFT. The electronic and structural properties of Li_3N was investigated within the frame work of the density functional theory (DFT) with the Perdew Burke-Ernzerhof (PBE) exchange-correlation functional, Vanderbilt (ultra soft) pseudopotentials and the plane wave basis set implemented in the Quantum-ESPRESSO program package. All calculations have been carried out with Quantum Espresso package. The total minimum energy calculation is performed as a function of cut-off energy and Monkhorst pack-grid size (K-points sampling), respectively fixing the other parameters constant. The total energy convergence test is achieved, at the energy cutoff 80 Ry for the energy cutoff case and at $8 \times 8 \times 8$ k-point grid size for the K-point sampling case. The total minimum energy is -63.37054774 Ry for the first case and -63.37056177 Ry for the second case. The total minimum force on Li_3N as a function of cutoff energy and Monkhorst-Pack grid is calculated by displacing Li atom by +0.05. Total force convergence test is achieved for the cutoff energy 80 Ry and for Monkhorst-Pack grid at286.3023306 $8 \times 8 \times 8$ k-point grid size. The numerical calculation shows that the equilibrium lattice constant is 3.501.

This value is in good agreement with existing experimental value which is 3.651 A.

In the case of investigating the band gap of Li_3N, we observed that indirect band gap of bulk Li_3N is changed to direct band gap of Li_3N. This change makes it interesting for applications in optoelectronics. Also, experimentally the band gap of Li_3N is about 2.0 eV and our numerical calculation shows 1.1 eV, which has 0.082 percent of error with the experimental value. Finally, the calculated DOS of Li_3N determines its electrical property. The calculated energy gap of Li_3N between the occupied and unoccupied energy levels in case of DOS is 1.1 eV and has 0.082 percent of error with experimental value. This value shows as this system is semiconductor.

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Name of Student: **kassa Adugna Gonfa** ID No. **S30302/10**

Graduate Program: **Summer, M.Sc.**

1. Course Work Performance

Course Code	Course Title	Cr. hr	Number Grade	Rank **	Remark
Phys699	**M.Sc. Thesis**	**6**	**75.54**	**Very good**	

** Ecellent, Very Good, Good, Satisfactory, Fail.

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email:kassaadugna120@gmail.com

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Jimma University

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