

PRESSURE INDUCED PHASE TRANSITION OF LaAlO_3

Submitted in partial fulfillment of the requirements for the award of

MASTER OF SCIENCE DEGREE IN PHYSICS

By

RAMAN S B

(40590004)



DEPARTMENT OF PHYSICS

SCHOOL OF SCIENCE AND HUMANITIES

SATHYABAMA

INSTITUTE OF SCIENCE TECHNOLOGY

(DEEMED TO BE UNIVERSITY)

Accredited with Grade “A” by NAAC

JEPPIAAR NAGAR, RAJIV GANDHI SALAI, CHENNAI - 600 119

APRIL - 2022



SATHYABAMA

INSTITUTE OF SCIENCE AND TECHNOLOGY

(DEEMED TO BE UNIVERSITY)

Accredited "A" Grade by NAAC | 12B Status by UGC | Approved by AICTE

www.sathyabama.ac.in

DEPARTMENT OF PHYSICS

BONAFIDE CERTIFICATE

This is to certify that this Project Report is the bonafide work of RAMAN S B (40590004) who carried out the project entitled **PRESSURE INDUCED PHASE TRANSITION OF LaAlO_3** under my supervision from NOV 2021 to APR 2022.

Internal Guide

(Dr.D.S.JAYALAKSHMI)

External

Guide

Head of the

Department

(Dr. S.

RAVICHANDRAN)

Submitted for Viva-voce Examination held on

Internal Examiner

External Examiner

DECLARATION

I RAMAN S B (Reg.No 40590004) hereby declare that the Project Report entitled **“PRESSURE INDUCED PHASE TRANSITION OF LaAlO_3 ”** done by me under the guidance of **Dr.D.S.JAYALAKSHMI, ASST. PROFESSOR, DEPARTMENT OF PHYSICS** at SATHYABAMA INSTITUTE OF SCIENCE AND TECHNOLOGY, CHENNAI is submitted in partial fulfillment of the requirements for the award of Master of Science degree in Physics.

DATE:

PLACE:

SIGNATURE OF THE CANDIDATE

ACKNOWLEDGEMENT

I am pleased to acknowledge my sincere thanks to the Board of Management of **SATHYABAMA** for their kind encouragement in doing this project and for completing it successfully. I am grateful to them.

I convey my thanks to the Dean, School of Science and Humanities and **Dr. S. RAVICHANDRAN**, Head of the Department, Dept. of Physics for providing me necessary support and details at the right time during the progressive reviews.

I would like to express my sincere and deep sense of gratitude to my Project Guide **Dr.D.S.JAYALAKSHMI** for her valuable guidance, suggestions and constant encouragement that paved way for the successful completion of my project work.

I wish to express my thanks to all Teaching and Non-teaching staff members of the Department of Physics who were helpful in anyways for the completion of the project.

RAMAN S B

Abstract

A computational investigation over structural and electronic properties of perovskite compound namely LaAlO_3 using WIEN2K code by means of Full-potential (FP) Linearized Augmented Plane Wave (LAPW) method using DFT (Density Functional Theory) have been analyzed under the effect of pressure to brief the trend of phase transition in the present compound. The compound is investigated up to the pressure of 9.068 GPa from the ambient condition. In this study, the cubic structural properties of the proposed compound are analyzed under pressure and initiated with $a = 7.2108$ bohr belong to the space group 51_P1 and 1000 K points with $R_{\text{MT}}^* K_{\text{Max}}$ is 7. From the analysis of Density of state (DoS) histograms profiles, it evidentially shows that the compound being an insulator by the increment in the band gap under the applied pressure. The structural phase transition occurs at the pressure value 6.318 GPa and compression of volume 15 % from the ambient condition. In this range of pressure, a closed contour are occur around La to Al and La to O atoms, It depicts that the formation of covalent bond between the mentioned atoms, may increases the stability of the compound. The optimized lattice parameter, the positional z-parameter, distance and angle between the atoms, Fermi energy, Density of States (DOSs) at Fermi Level, electronic specific heat coefficient and the distance between La(Al)–Al(O) and La–O atoms at equilibrium lattice configuration ($V/V_0=1$) and under compressions ($V/V_0=0.95$, $V/V_0=0.9$, $V/V_0=0.85$, $V/V_0=0.8$) are analyzed. High pressure band structure calculations reveal the possibility of Electronic Topological Transition (ETT) in this compound at $V/V_0=0.85$ or 6.318 GPa.

TABLE OF CONTENTS

CHAPTER NO	TITLE	PAGE NO
	ABSTRACT	v
	LIST OF TABLE	vi
	LIST OF FIGURES	vi
	LIST OF SYMBOLS	x
1	INTRODUCTION	1
	1.1 DENSITY FUNCTIONAL THEORY	2
	1.2 FULL - POTENTIAL LINEARIZED AUGMENTED PLANE WAVE (FP-LAPW) METHOD	3
	1.3 WIEN2K CODE	4
2	2.1 AIM	6

	2.2 SCOPE	6
	2.3 MATERIAL	7
	2.3.1 LaAlO₃ COMPOUND	7
3	3. COMPUTATIONAL DETAILS	8
	3.1 WIEN2k	8
	3.3 APPLICATIONS OF WIEN2K	9
	3.4 FLOW OF COMPUTATIONAL WORK	12
4	4. RESULT AND DISCUSSION	13
	4.1 Pressure study in LaAlO₃ compound	13
5	Summary	26
	Conclusion	27
	Reference	28

LIST OF TABLES

TABLE NO	TITLE	Page NO
4.1	structural and electronic properties of LaAlO ₃ compound under compression	15
4.2	distance between the atoms of LaAlO ₃	17

LIST OF FIGURES

FIGURE NO	TITLE	PAGE NO
4.1	LaAlO ₃ structure	14
4.2	LaAlO ₃ structure after phase transition	14
4.3	Figure volume optimization	16
4.4	Density of states of LaAlO ₃ at V/V* (a) 1 (b) 0.95 (c) 0.90 (d) 0.85 (e) 0.80	18
4.5	Electron density plot of LaAlO ₃ at V/V* (a) 1 (b) 0.95 (c) 0.90 (d) 0.85 (e) 0.80	21
4.6	Band structure of LaAlO ₃ at V/V* (a) 1 (b) 0.95 (c) 0.90 (d) 0.85 (e) 0.80	23

LIST OF SYMBOLS AND ABBREVIATIONS

E_F	-	Fermi energy
F_L	-	Fermi level
$F_{HK} [\rho]$	-	Hohenberg Kohn density functional
$N(E_F)$	-	DOS Fermi level
$n(r)$	-	electron density
BZ	-	Brillouine Zone
DFT	-	Density Functional Theory
DOS	-	Density of states
FP-(L)APW	-	Full Potential - (Linearized) Augmented Plane Wave
GGA	-	Generalized gradient Approximation
GUI	-	Graphical User Interface
LDA	-	Local Density Approximation
LMTO	-	Linear Muffin Tin Orbital
OPW	-	Orthogonalized Plane Wave
RMT	-	Radius of Muffin Tin spheres
EPM	-	Empirical Pseudo potential Method

CHAPTER 1

1.Introduction

in order to reduce the probabilities of mistakes in experiment, it is very important to understand the nature of the material to the modern hypothetical compound. computer stimulation allows us to study the complex material that contain many electrons and act as a key element in the process to analysis and to explain the complex stages or to plan future experiments in a rational way. as a result the stimulation method is more efficient to comparing with old trial an mistakes method where we improve a material through synthesizing, characterizing and functional analyzing. Quantum mechanics governs the electronic structure which is responsible for the properties of the system, along with the relative stability, chemical bonding, relaxation of the atoms, phase transitions, electrical, mechanical, magnetic behavior, and so forth.. (Schwarz k et al 2002). The well-established scheme to calculate the electronic properties of solids is density functional theory (DFT), DFT is a completely familiar computational quantum mechanical modeling method used in physics, chemistry and material science of many body systems, in a specific atom, molecules and the condensed phases. it is based on electron density instead of wave function (Hartree Fock), and it treats both exchange and correlation. Many computer codes are available in which our compounds are studied under WIEN2K code. Majorities of interactions in solids depend critically on the interatomic distance. The application of pressure changes the inter-atomic distance and alter the structure and electronic properties without introducing any chemical complexity and preserving the physical complexity to a minimum. consequently, high pressure techniques. have been extensively used in recent years to explore the physical states of solids, to create new ground states in solids, to check theoretical models and to help develop new theories. as an example, there are more naturally non superconducting elements that have been turned into superconductors via the application of pressure in the last half-century than naturally taking place elemental superconductors. This makes high.

pressure system open to the computational study.

1.1 DENSITY FUNCTIONAL THEORY

Over the past few decades, density functional theory (DFT) has been most successful, widely used method in condensed-matter physics, computational physics and quantum chemistry to describe properties of condensed matter systems, which include not only standard bulk materials but also complex materials including molecules, proteins, interfaces and nanoparticles. the main concept of DFT is to explain a many-body interacting gadget via its particle density and not through its many body wave function. Its significance is to reduce the $3N$ degrees of freedom of the N body system to only 3 spatial coordinates through its particle density. Its foundation is the well-known Hohenberg-Kohn (HK) theorem, which claims that all properties of a gadget may be taken into consideration to be unique functional of its ground state density. collectively with the Born-Oppenheimer (BO) approximation and Kohn-Sham (KS) equation, practical accurate DFT calculations have been made possible via approximations for the so-called exchange-correlation (XC) potential, which describes the effects of the Pauli principle and the Coulomb capability past a pure electrostatic interaction of the electrons. on the grounds that it is impossible to calculate the exact XC potential (by solving the numerous-body problem exactly), a common approximation is the so-called local density approximation (LDA) which locally substitutes the XC energy density of an inhomogeneous system through that of a homogeneous electron gas evaluated at the local density. in many instances the outcomes of DFT calculations for condensed-matter systems agreed quite satisfactorily with experimental data, especially with better approximations for the XC energy functional since the 1990s. also, the computational expenses have been relatively low in comparison to traditional methods which have been based on the complex many-electron wave function, such as Hartree-Fock theory and its descendants. despite the improvements in DFT, there are nonetheless difficulties in the usage of DFT to correctly describe intermolecular interactions; charge transfer

excitations; transition states, international potential energy surfaces and some other strongly correlated systems; and in calculations of the band gap of some semiconductors.

There are several different schemes to the calculation of the independent particle electronic states in solids where boundary conditions are applied. They are basically classified into three types: (i) Plane wave codes are Quantum ESPRESSO, ABINIT, VASP, etc., (l) Localized atomic orbitals are CRYSTAL, SIESTA, etc, (m) augmented plane wave codes are LMTO, FLEUR, WIEN2K. Of which, WIEN2K code is based on the full potential (linearized) augmented plane wave (LAPW)+ local orbitals (LO) method.

1.2 FULL - POTENTIAL LINEARIZED AUGMENTED PLANE WAVE (FP-LAPW) METHOD

The accuracy of the LAPW+ lo method can be further stepped forward by means of using the full potential (FP). The potential approximated to be spherically inside the muffin-tins, while in the interstitial region the potential is ready to be constant. it is a method used to simulate the electronic properties of materials on the basis of DFT. This method has been successfully applied to study structural phase transitions of certain semiconductors, which will increase the number of plane waves in the basis set, in order to lower the structural properties of systems accurately. The shape of the charge density is taken into account with high accuracy in this method, the unit cell is divided into two regions (i) Muffin tin radius (ii) interstitial region (iii) total spherically averaged potential

In FP-LAPW method, both the potential and charge density are expanded into lattice harmonics inside each atomic sphere and as a Fourier series in the interstitial region.

therefore, the plane wave solves the Schrodinger equation in interstitial place, and the product of radial solution times the round harmonic solution solve the Schrodinger equation in the muffin-tin region.

1.3 WIEN2K CODE

WIEN2K is a full-potential all-electron code developed by Blaha (2001) to study the properties of crystal. It consists of many independent F90 programs, which might be linked together via C-shell scripts. The code is based on the Kohn-sham formalism of DFT. The code initially starts from structure generation document containing information on space group, lattice parameters, atomic species, atomic position, muffin tin radii, etc. based totally on the input values the materials are initialized through step by step process: (i) NN distance- check for overlapping spheres, coordination numbers, nearest neighbor distances and thus decide the atomic sphere radi. (i) SGROUP- calculates the point and space groups for the given structure. (ii) SYMMETRY- check the symmetry operations and determines the point group of the individual atomic sites. (iii) LSTART- generates atomic densities for all atoms. (iv) KGEN- generates a k-mesh in the Brillouin zone, (v) DSTART-generates a starting density for the SCF cycle via superposition of atomic densities

The self-consistent is an iterative approach that includes selecting the Schrödinger equation to achieve a more accurate set orbitals after which solving the Schrödinger equation again with theses until the results converge. The scf cycle starts with LAPWO where it computes the total potential as the sum of the coulomb and the exchange correlation potential. subsequent LAPW1 sets the Hamiltonian and the overlap matrix and finds the Eigen values and Eigen vectors of the valence states by diagonalization of the Kohn-Sham equation. followed by LAPW2 which generates valence charge density and computes Fermi energy.

The states and energies of the core electron are calculated one at a time in a ordinary atomic calculation in the LCORE, which results in the overall core density. both core and valence density mixed to give overall density. since the density often, differs a lot from the old density, they are mixed by MIXER to avoid huge fluctuations among iterations that could leads to divergence. once the end of the cycle is reached, WIEN2K checks for the new and new density, if they vary from each other a new iteration is started with new density. This procedure is repeated until old and new density is consistent. LAPWSO calculation takes place only if we include spin-orbit

CHAPTER 2

2.1 AIM

The main aim of this work is to study the structural property of compounds LaAlO_3 with space group 51_P1 under pressure by means of Full Potential - Linearized Augmented Plane Wave (FP-LAPW) method as implemented in WIEN2K code. The motive of the study is to investigate the structural transition and analyze the conductivity nature of the compounds under pressure.

2.2 SCOPE

Important for the understanding of the properties of perovskite compound is a detailed knowledge of structural parameters and with superconducting behavior. The electronic structure and physical properties of the materials can be tuned by pressure with various range in the compounds.

Some of the recent research of compounds under pressure are as follows:

BaMn_2As_2 , metallization at 5.8 GPa with sharp fall in resistivity indicating a possibility of superconductivity (T. Satya et al.,). The CaFe_2As_2 compound precise nature of the crystallographic structure of the superconducting phase is under debate but the CT phase is obtained under hydrostatic pressure condition (Tuson Park et al.,)..

BaFe_2As_2 compound revealed a bulk superconductivity under a critical pressure of 2.8 GPa (Awadhesh Mani et al.,). EuCo_2As_2 compound changed from tetragonal phase to collapsed tetragonal phase at 4.7 GPa (Matthew Bishop et al.,). SrFe_2As_2 compound loses its resistivity and superconductivity occurs at 3 GPa (T_c -29 K).

2.3 MATERIAL

2.3.1 LaAlO₃ COMPOUND

LaAlO₃ is interesting to study for several reasons. First, at ambient conditions the rhom-bohedral deviation from the ideal perovskite can be approximated by a simple tilt of the AlO₆ octahedra. As a consequence, for LaAlO₃ one might well expect to be able to describe the eventual phase transition in a quantitative way—in contrast to the existing qualitative description of the pressure-induced phonon softening in ATiO₃ (A = Ba, Pb, Na_{0.5}Bi_{0.5}) which is driven by tilting and cation displacement. Further interest in LaAlO₃ stems from the fact that it is widely used as a substrate for thin-film growth of perovskite structures or structures containing perovskite-type structural blocks like high-temperature superconductors. It is well known that the deposition of thin films can lead to large strain effects at the film–substrate interface and, therefore, it is of interest to get a better understanding of the effect of pressure on LaAlO₃.

CHAPTER 3

3. COMPUTATIONAL DETAILS

3.1 WIEN2k

WIEN2k is one of the most efficient and dependable simulation codes available. This code was used to perform all of the computational work on lanthanide intermetallic compounds. Blaha et al. at the Institute for Materialchemie, Technical University of Wien, Austria, created WIEN2k, a full-potential all-electron code. WIEN2k is made up of a number of separate F90 programmes that are linked together using C-shell scripts. The code is based on the DFT formalism of Kohn-Sham.

We saw how to simplify a complex problem with many interacting particles to a Schrodinger wave equation in the previous chapter. To solve these equations, we must first create the effective Hamiltonian operator, which is based on the electronic system's electron density. The flow chart depicts the method by which the Schrodinger wave problem is solved in Code WIEN2k.

WIEN2k CODE

The following are the considerations that were made in the construction of the new Wien2k package that are needed for a current computer code.

a) Reliability

A well-balanced basis set, which contains numerical radial functions that are calculated in each iteration cycle, is used to achieve this. As a result, these functions adapt to charge transfer or hybridization processes and are accurate near the nucleus. It's an all- electron, full-potential approach. The treatment of relativistic effects (including spin orbit coupling) is akin to solving Dirac's equation. The periodic table's atoms can all be handled.

B) Efficiency and Performance

This condition is best satisfied by the new mixed base APW+lo/LAPW. Smaller matrix sizes save computer time, allowing for the study of bigger systems.

c) Parallelization

If the memory need is greater than that available on a single CPU, the programme can run in parallel, either in a coarse grain version where each k-point is computed on a single processor or in a fine grain scheme where each k-point is computed on several processors.

d) Architecture

During the installation of the programme package, efficient algorithms and libraries are employed based on the architecture.

e) Portability

It necessitates the adoption of industry standards whenever possible, such as FORTRAN90, MPI, BLAS, SCALAPACK, and so on.

g) User friendliness

W2web, a web-based graphical user interface (GUI), is used to do this. The application package includes an exhaustive User's Guide as well as an automatic selection of default choices.

3.3 APPLICATIONS OF WIEN2K

So far, problems investigated in QM calculations utilising the LAPW approach (used in various versions of the Wien code) have included insulators, semiconductors, (transition) metals up to f -electron systems, and intermetallic compounds. Below is a brief overview of a number of uses.

i) Calculations of band structure and density of states (DOS)

The energy band structure and matching density of states are important factors in determining a system's electronic structure. Their examination reveals information on the electric properties (metal, insulator, or semiconductor) as well as chemical bonding.

The strength of interactions between the orbitals of the constituent atoms can be inferred from site decomposed partial densities of states. In the context of photoelectron spectra, the band structure is also useful.

ii) Electron densities

In DFT, the electron density is the most important quantity. The static structural factors can be easily computed using the Fourier transform, and the results may be compared to experimental X-ray diffraction data.

iii) Electric field gradients (EFG)

The EFG may be calculated from first principles since it is uniquely characterised by charge distribution and consequently electron density. The nuclear quadrupole interaction (NQI) determines the anisotropy of charge density distribution close to the nucleus, which can be studied by nuclear magnetic resonance (NMR), nuclear quadrupole resonance (NQR), Mossbauer, or perturbed angular correlation (PAC) experiments.

iv) Total energy and phase transitions

With total energy in hand, the relative stability of distinct phases can be calculated by holding as many parameters constant as feasible to balance out systematic mistakes.

v) Forces and structural optimization

When atoms occupy generic places that are not determined by crystal symmetry, understanding the forces acting on them aids in the optimization of structural parameters. In Wien2k, forces can be calculated and are vital for such optimizations.

vi) Spectra

Using partial densities of states and transition probabilities between a valence and a core state, photoelectron spectra, X-ray emission, and absorption spectra can be estimated. The local binding situation of the atom whose core state is involved is revealed by such spectra. Electronic response can be used to calculate optical spectra and related quantities such as the energy dependence of the real and imaginary parts of the dielectric constant, which is then used to calculate absorption coefficient, refractive index, electron energy loss spectrum, and reflectivity using the Kramers-Kroening relation.

vii) Others:

Many features, such as chemical bonding, structural stability, high-pressure phases, Jahn–Teller distortions, charge distribution, phase transitions, ferroelectric, ferroelectric, or elastic properties, have been explored using WIEN2k for a wide range of structures. In magnetic solids, the roles of spin and orbital magnetic moments, magnetic ordering (ferro-, ferri-, antiferro-magnetic), and meta-magnetism were studied (including intermetallic compounds). Optical, core-level, photoelectron, Mossbauer, and NMR spectra have all benefited from LAPW computations.

Hyperfine or crystal fields, the magneto-optical Kerr effect, and electric field gradients are all covered. By investigating a super-cell 2x2x2 (or larger), i.e. doubling the original unit cell in all three dimensions, flaws, such as impurities, can be represented. When an impurity atom replaces one of the atoms in this huge unit cell, the nearby atoms can relax into new equilibrium states.

An isolated impurity can be approximated by repeating such a super-cell on a regular basis. Surfaces and their interactions with atoms or molecules can also be simulated using super-cells. Regardless of whether or not they can be built in reality, hypothetical or artificial structures can be evaluated and their properties calculated. These computations can be used to anticipate a system's attribute (e.g., insulator or metal) or to determine its magnetic structure.

It is possible to mimic changes in a system due to deformations, pressure, or substitutes. Using the WIEN2k programme, density of states (DOS), partial density of states (PDOS) of constituent atoms, electronic band structure, and frequency dependence of linear optical properties such as real and imaginary part of dielectric constant, refractive index, reflectivity, and electron energy loss spectra (EELS) for PbMoO_4 , BaWO_4 , and $\text{NaBi}(\text{WO}_4)_2$ were calculated.

3.4 FLOW OF COMPUTATIONAL WORK

In this paper, the WIEN2k algorithm is used to calculate the electrical structure of solids using the Full Potential Linearized Augmented Plane Wave technique. Generalized gradient approximation (GGA) and local density approximation are used to calculate the exchange and correlation energy (LDA). Monkhorst Pack $10 \times 10 \times 10$ k-points were used for the Brillion zone integration. The basis function was stretched up to $\text{RMT} \times K_{\text{max}} = 7$ in order to obtain convergence. While the charge density is Fourier expanded up to $G_{\text{max}}=12$, the maximum value for partial waves inside the atomic sphere is $l_{\text{max}}=10$.

The estimated lattice parameter will be used for structure file construction, initialization, and self-consistent field cycle performance. To calculate the band structure of ternary cubic compounds, a structure file is first created using the optimal lattice constant. Then, using the original binary chemical, a $2 \times 2 \times 2$ supercell is produced, and the ternary addition is performed. The calculations for the ternary compound are now carried out as shown in the flowchart.

CHAPTER 4

4. RESULT AND DISCUSSION

4.1 Pressure study in LaAlO₃ compound

All calculation reported here have been performed using full-potential linearized augmented plane wave code WIEN2K (Blaha, 2001), using generalized gradient approximation (GGA), incorporated in code for the exchange correlation potential. The crystal structure of LaAlO₃ is cubic and space group is 51_P1 . The muffin tin radii for the ground state and the high-pressure calculation for LaAlO₃ have been done. The structure of LaAlO₃ is shown in Fig.4.1

The basis set corresponding to RKmax was used for all calculations. The total energy and density of states (DOS) calculation are carried out with more than 100 K points in the irreducible Brillouin zone to attain good energy and charge convergence. The DOS has been calculated using the tetragonal integration method. The total energy of the given system is obtained and then fitted into the Birch-Murnaghan equation of state shown in Fig 4.2.

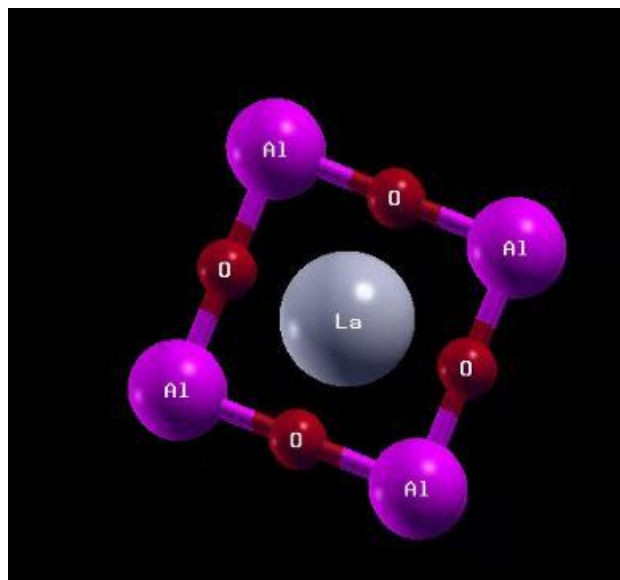


Figure 4.1 LaAlO₃ structure

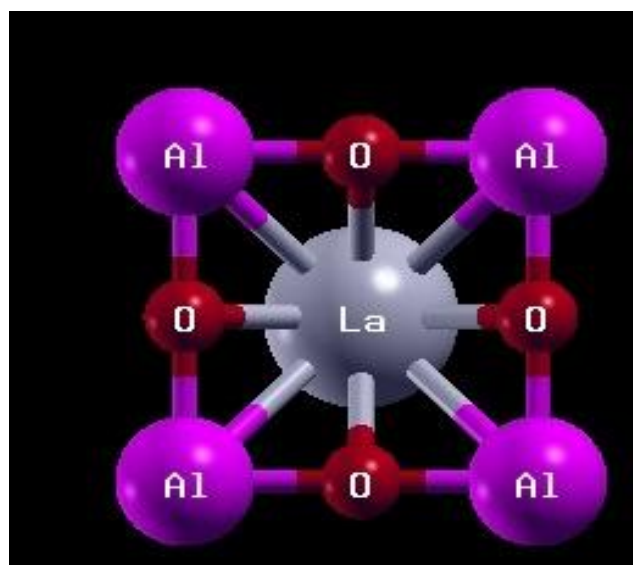


Figure 4.2 LaAlO₃ structure after phase transition at 6.318 GPa

Table 4.1 structural and electronic properties of LaAlO₃ compound under compression

V/V* ratio	1	V/V*=0.95	V/V*=0.90	V/V*=0.85	V/V*=0.80
<u>a(side lenght)</u> <u>bohr</u>	7.2108	7.0885	6.9619	6.8305	6.6938
<u>Volume (V)</u>	374.926	356.180	337.298	318.681	299.928
Space group	51_P1	51_P1	51_P1	51_P1	51_P1
Band gap(ev)	3.668	3.782	3.886	3.920	3.933
DOS	0.62270	0.67104	0.73121	0.77262	0.85126
FE	8.65	7.82	5.07	2.50	1.55
Pressure(GPa)	0.674	2.978	4.676	6.318	9.068

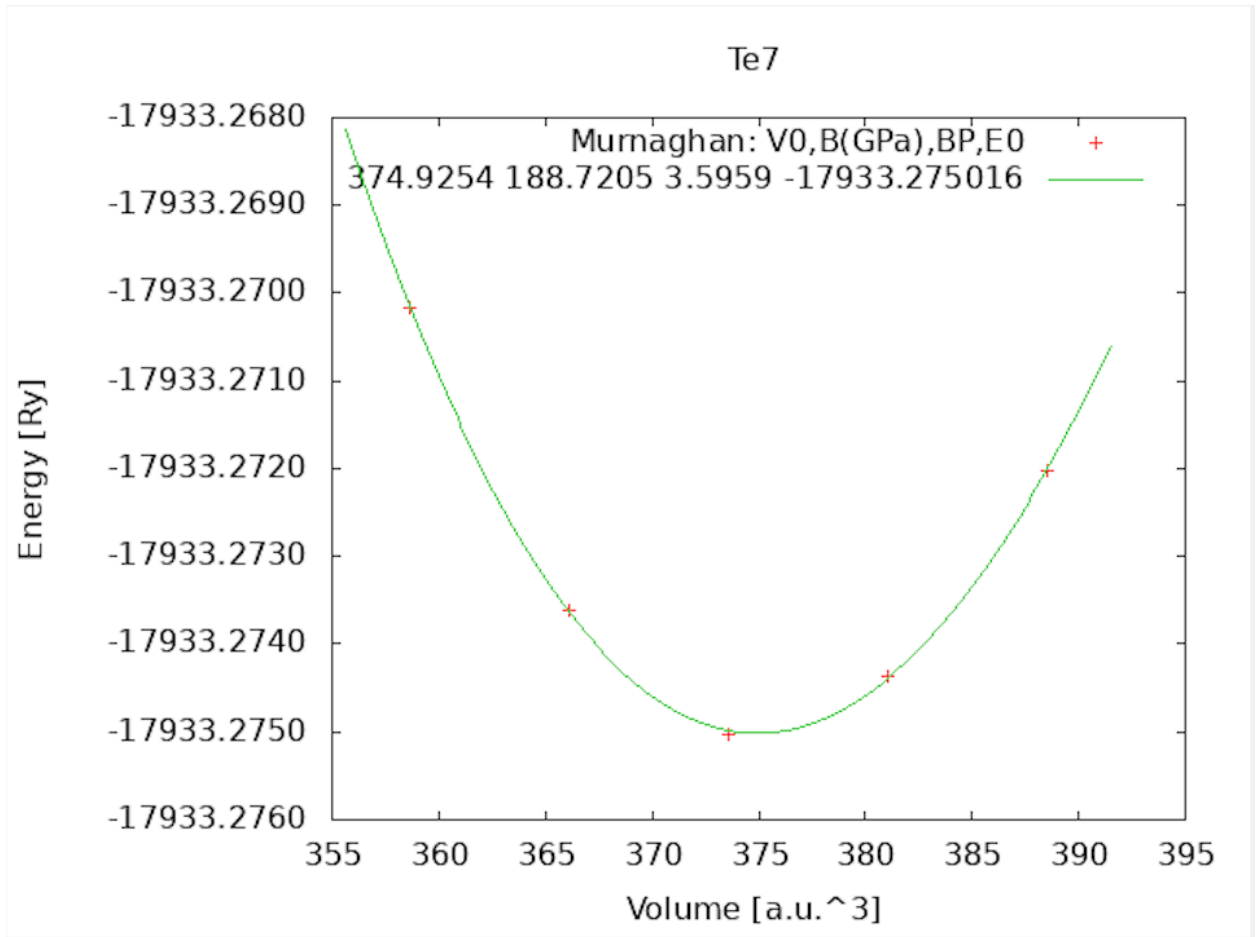


Figure 4.3 volume optimization

External pressure is applied to the compound is applied to the compound for various V/V_0 and the corresponding pressure experienced by the compound is obtained from the volume derivative of the Birch-Murnaghan EOS. As shown in the table 4.1, the DOS and FE does increase and decrease respectively due the pressure increase and there is increase in the band gap that result in the compound being an insulator for all the applied pressure. As the inward pressure increases from 0.674 GPa to 9.068 GPa we can observe DOS value also increases from 0.62270 to 0.85126 as expected, the FE decreases from 8.65 eV

to 1.55eV as the pressure increases. There is increase in band gap from 3.668 to 3.933 even when the volume of the compound is decreasing due to the increase in pressure

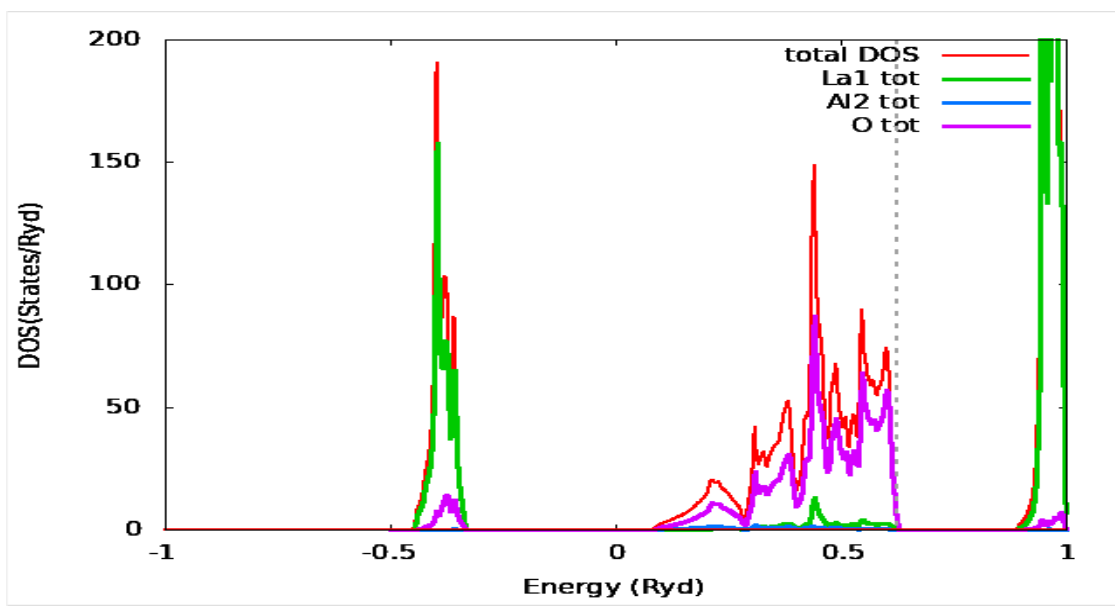
Table 4.2 distance between the atoms of LaAlO₃

V/V* ratio	1	0.95	0.90	0.85	0.80
Al-O	3.6054	3.5443	3.4810	3.4153	3.3469
La-Al	6.2448	6.1389	6.0292	5.9154	5.7971
La-O	5.0988	5.0124	4.9228	4.8299	4.7333
Angle Al-La-O	N/A	N/A	N/A	35.264	35.264

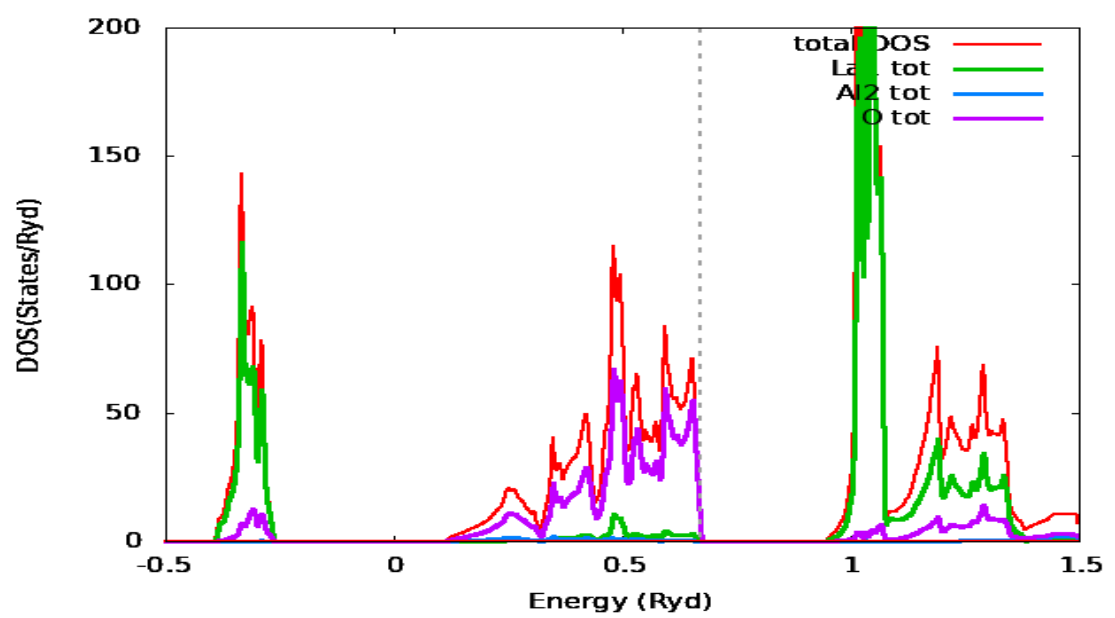
From the table 4.2, the structure of LaAlO₃ changes after V/V*=0.9. The distance between the atoms(bond length) decreases as the pressure increases between Al-O and La-Al and La-O

The angle between the atoms(Al-La-O) remain the same for the V/V* values 0.85 to 0.8

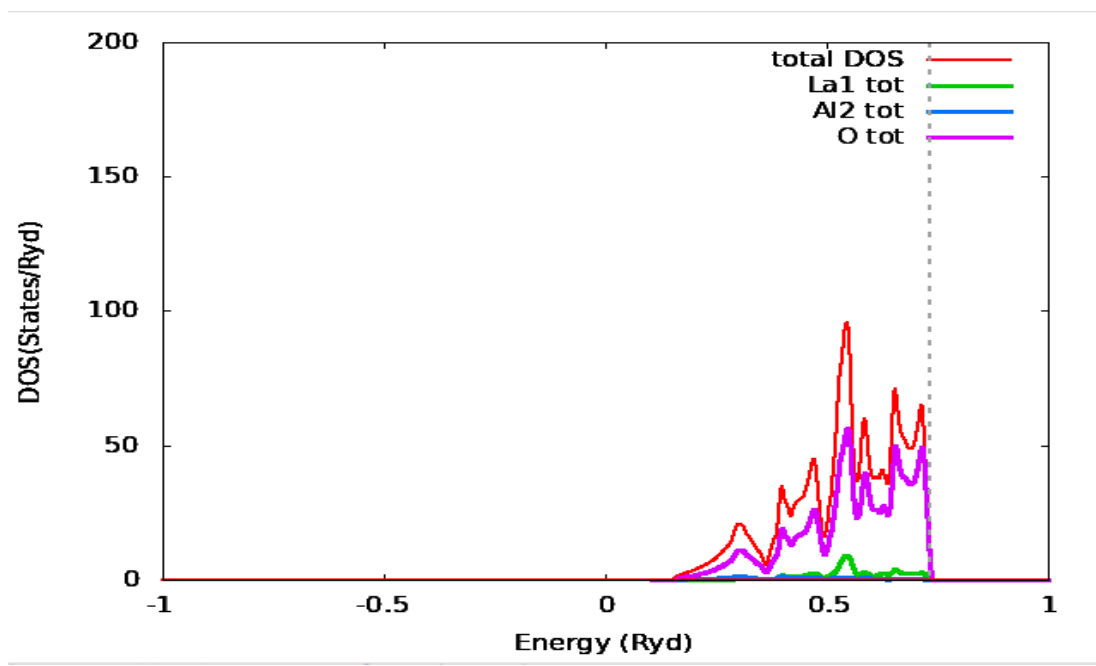
We can observe a phase transition



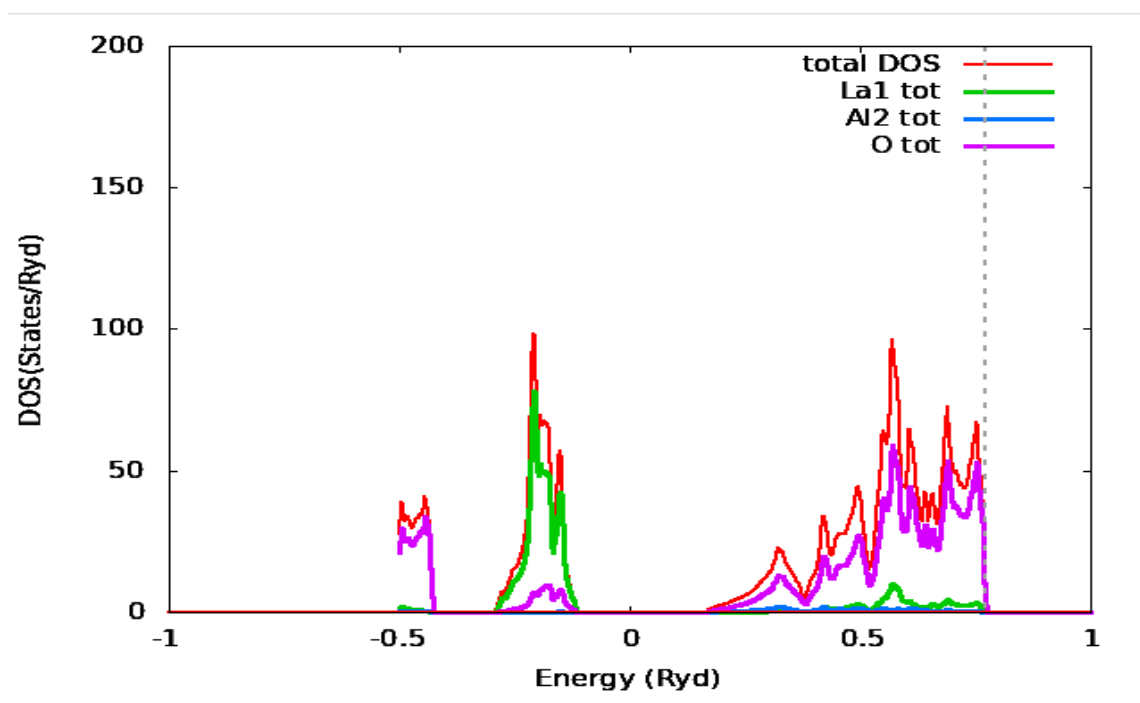
(a)



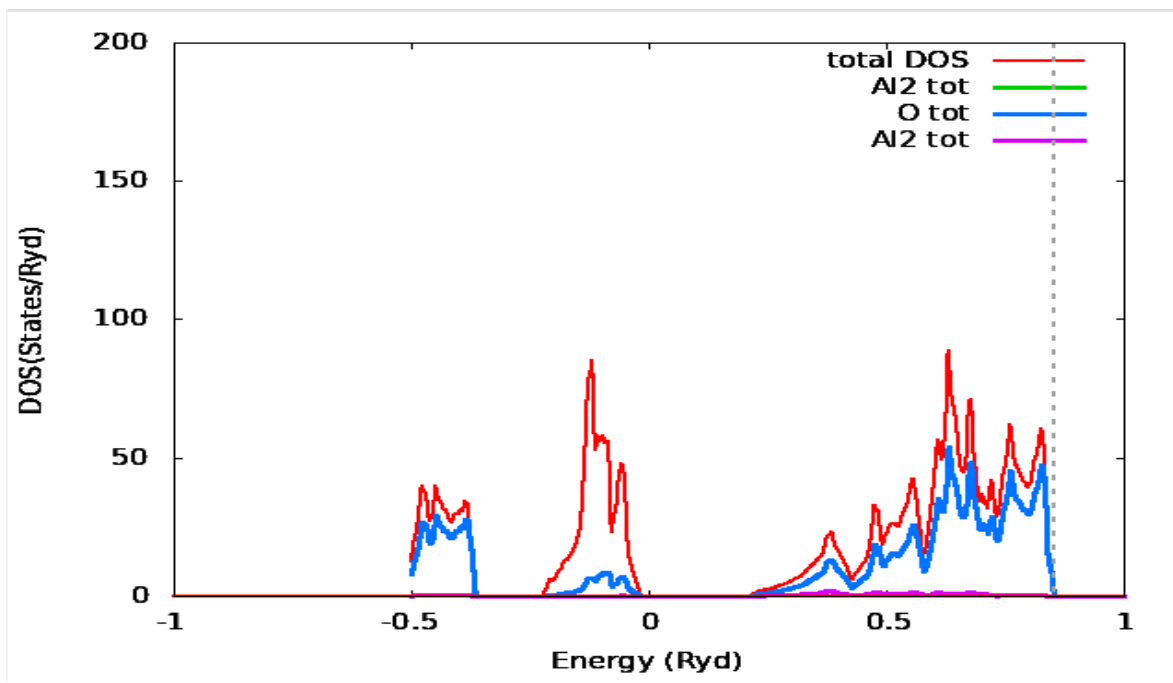
(b)



(c)

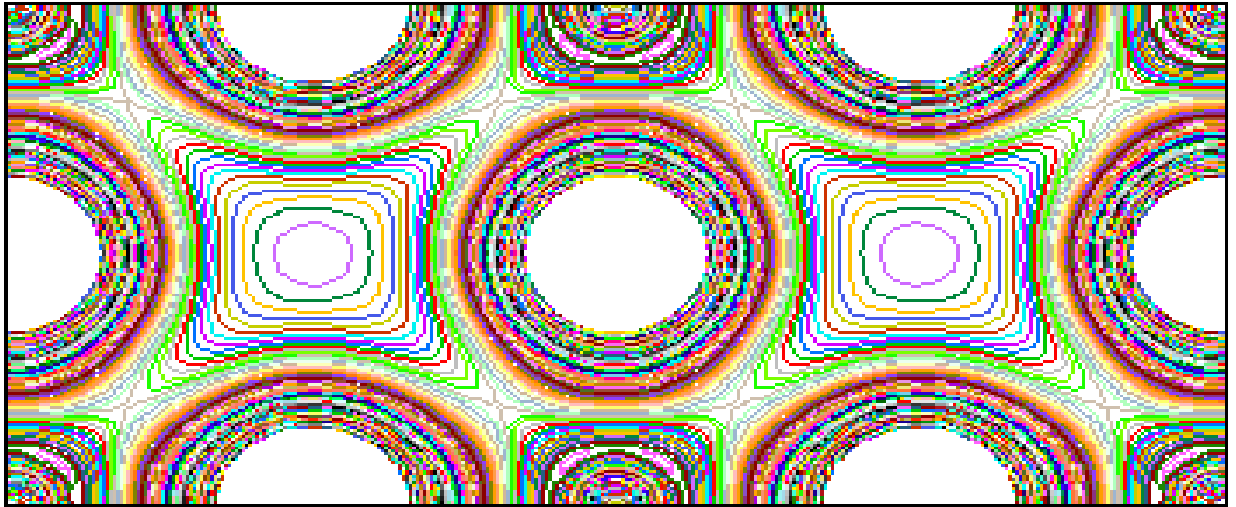


(d)

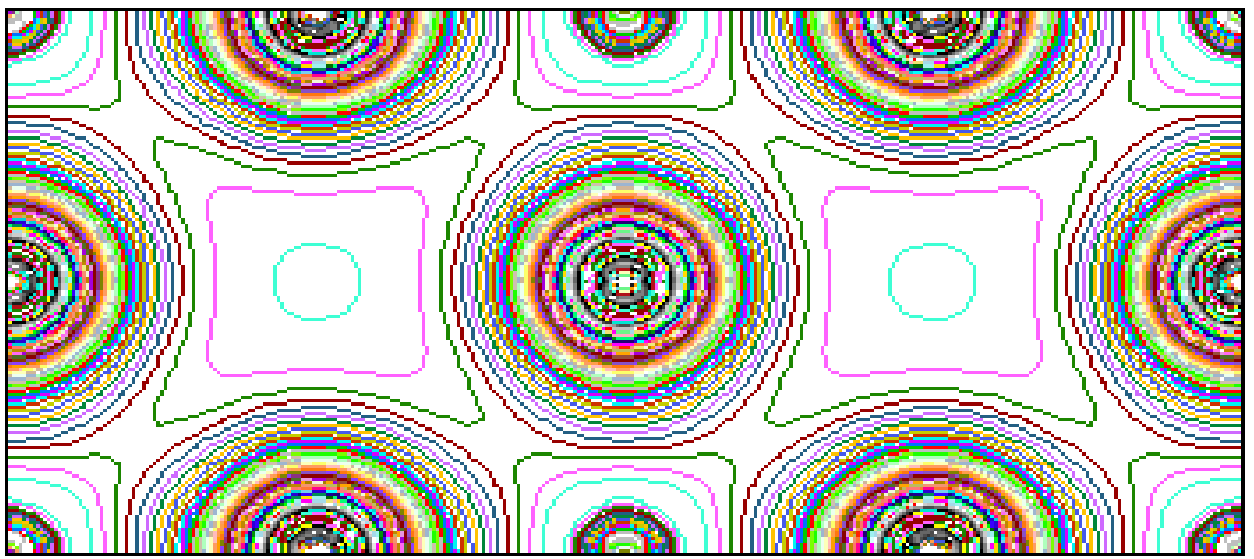


(e)

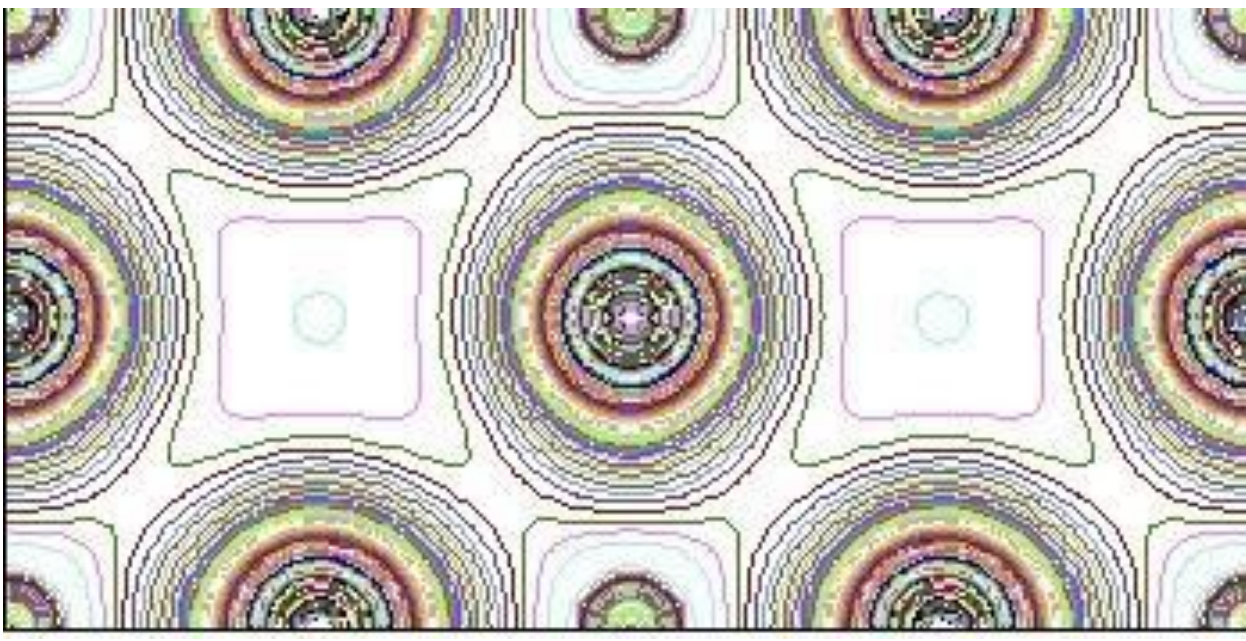
Figure 4.4 Density of states of LaAlO3 at V/V^* (a) 1 (b) 0.95 (c) 0.90 (d) 0.85 (e) 0.80



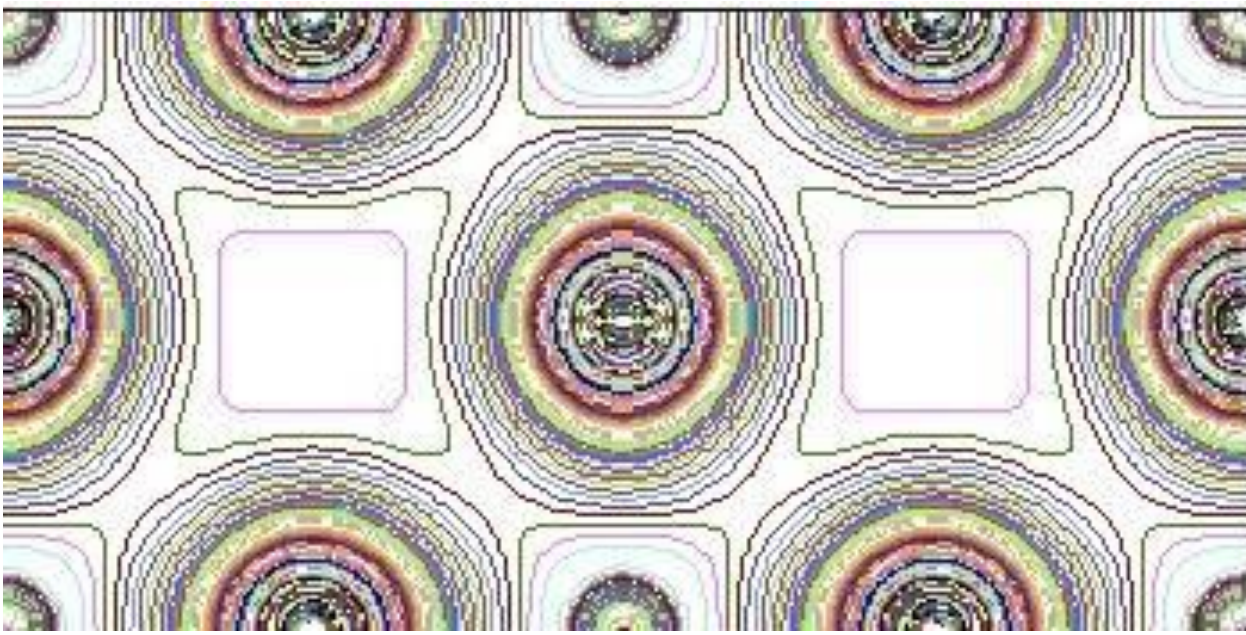
(a)



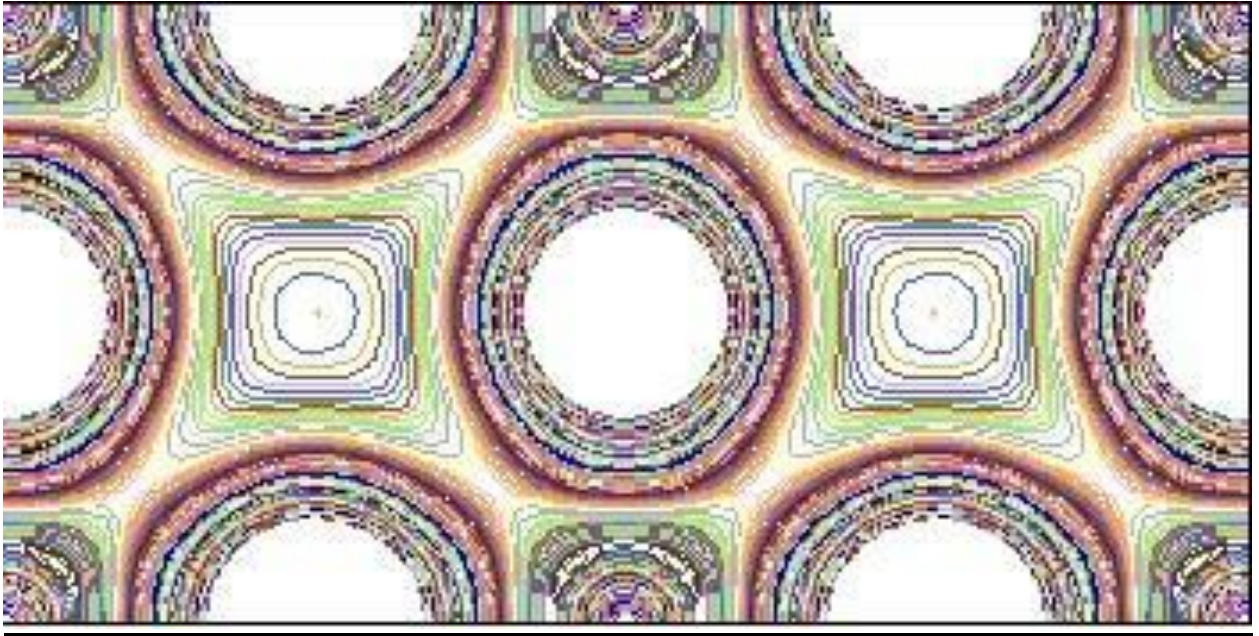
(b)



(c)

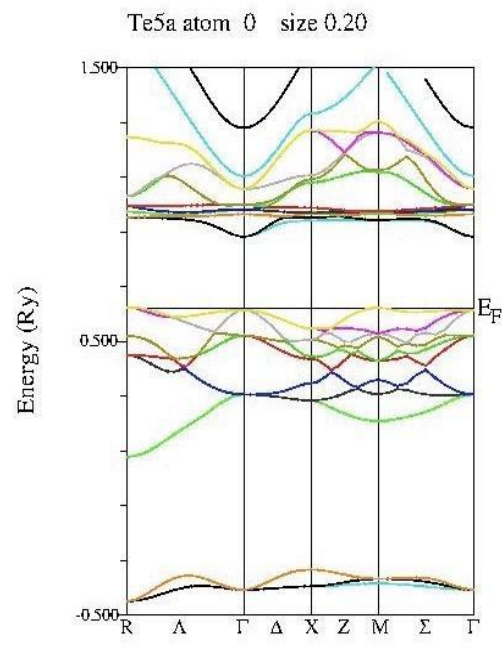


(d)

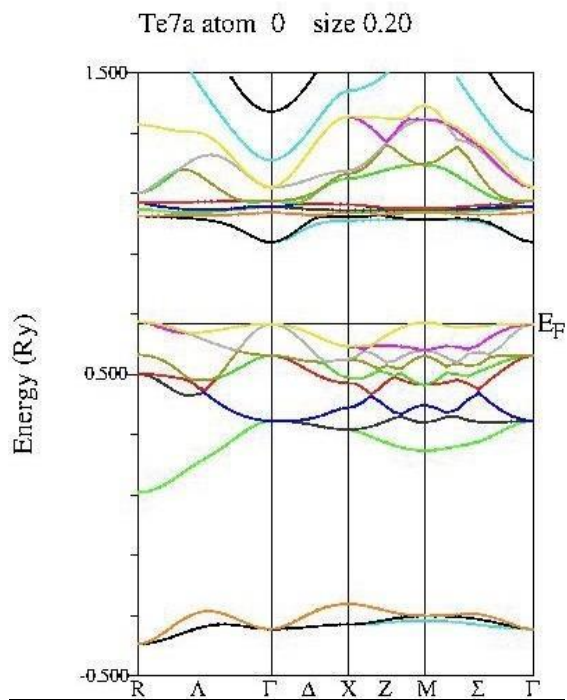


(e)

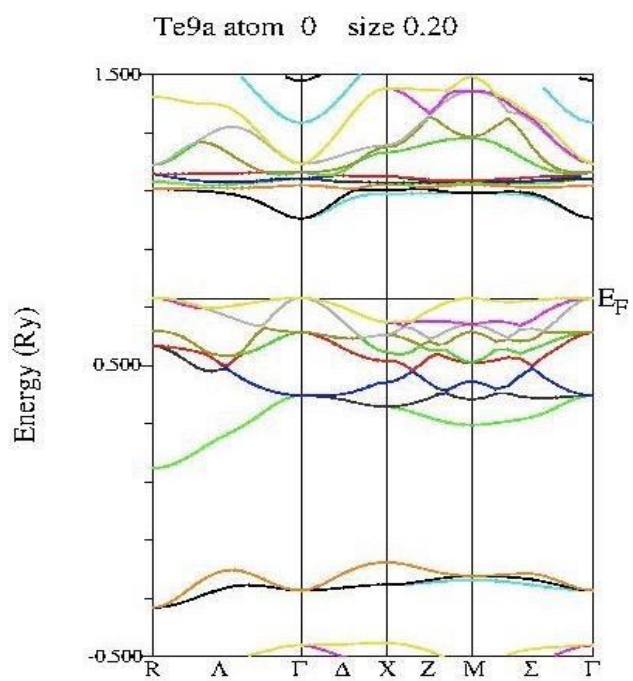
Figure 4.5 electron density plot of LaAlO₃ at V/V^* (a) 1 (b) 0.95 (c) 0.90 (d) 0.85 (e) 0.80



(a)



(b)



(c)

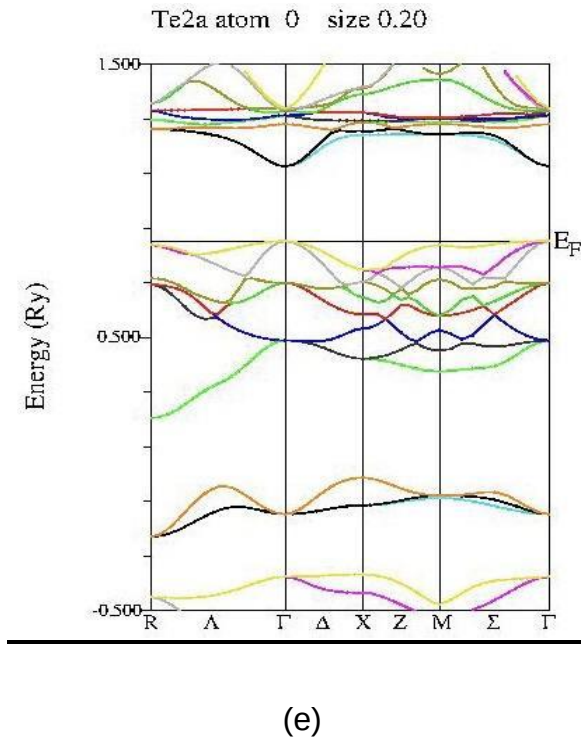
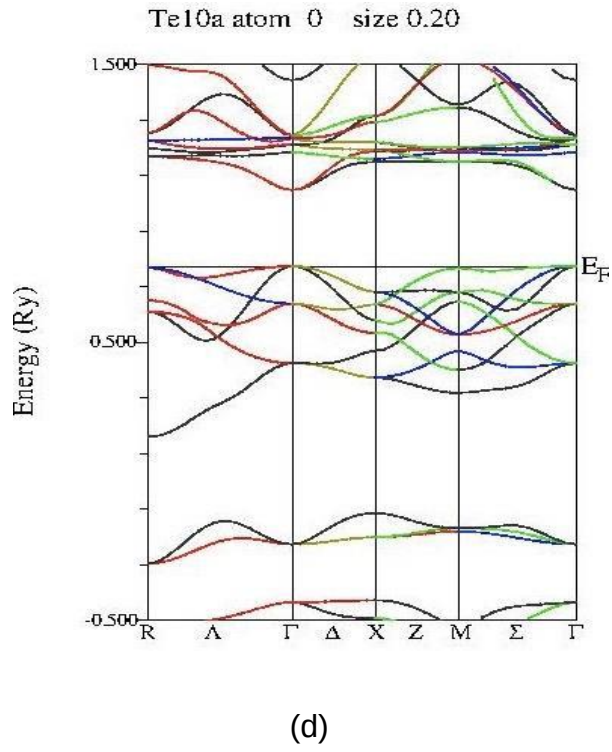


Figure 4.6 Band structure of LaAlO_3 at V/V^* (a) 1 (b) 0.95 (c) 0.90 (d) 0.85 (e) 0.80

Summary

The perovskite namely LaAlO_3 which are cubic in structure and space group is 51_P1 is studied under the Full Potential Linearized Augmented Plane Wave (FP-LAPW) method as implemented in the WIEN2K code. The compound is investigated up to the pressure of 9.068 GPa from the ambient condition. In this study, the cubic structural properties of the proposed compound are analyzed under pressure and initiated with $a = 7.2108$ bohr belong to the space group 51_P1 and 1000 K points with $R_{\text{MT}}^* K_{\text{Max}}$ is 7. From the analysis of Density of state (DoS) histograms profiles, it evidentially shows that the compound being an insulator by the increment in the band gap under the applied pressure. The structural phase transition occurs at the pressure value 6.318 GPa and compression of volume 15 % from the ambient condition. In this range of pressure, a closed contour is occur around La to Al and La to O atoms, It depicts that the formation of covalent bond between the mentioned atoms, may increases the stability of the compound. The optimized lattice parameter, the positional z-parameter, distance and angle between the atoms, Fermi energy, Density of States (DOSs) at Fermi Level, electronic specific heat coefficient and the distance between La(Al)–Al(O) and La–O atoms at equilibrium lattice configuration ($V/V_0=1$) and under compressions ($V/V_0=0.95$, $V/V_0=0.9$, $V/V_0=0.85$, $V/V_0=0.8$) are analyzed. High pressure band structure calculations reveal the possibility of Electronic Topological Transition (ETT) in this compound at $V/V_0=0.85$ or 6.318 GPa.

CONCLUSION

- The density of state (DOS) increases as the pressure increase
- The fermi energy FE does decrease respectively due the pressure increase
- there is increase in the band gap that result in the compound being an insulator for all the applied pressure
- As we can see the structure of LaAlO_3 in the figure 4.2 it changes at $V/V^*=0.85$ or at the pressure 6.318, which indicates that at the that pressure the compound becomes more stable
- There is a formation of new bonds between the atoms La and O
- The angle between the atoms (Al-La-O) remain the same for the V/V^* values 0.85 to 0.8
- We observe a phase transition

Reference

- [1] Rao, R.S., Majumdar, C.K., Shastry, B.S. et al. Effect of correlation on the band structure of cerium. *Pramana - J. Phys* 4, 45 (1975).
- [2] Blaha P., et al. (2001), WIEN2K, University Wien, Austria.
- [3] Bouvier, Pierre, and Jens Kreisel. "Pressure-induced phase transition in LaAlO₃." *Journal of Physics: Condensed Matter* 14.15 (2002): 3981.
- [4] Zhao, J., N. L. Ross, and R. J. Angel. "Polyhedral control of the rhombohedral to cubic phase transition in LaAlO₃ perovskite." *Journal of Physics: Condensed Matter* 16.47 (2004): 8763.
- [5] Zhao J, Ross NL, Angel RJ. Polyhedral control of the rhombohedral to cubic phase transition in LaAlO₃ perovskite. *Journal of Physics: Condensed Matter*. 2004 Nov 12;16(47):8763.
- [6] Behrendt, Mirosław, et al. "Influence of charge transfer state on Eu³⁺ luminescence in LaAlO₃, by high pressure spectroscopy." *Optical Materials* 63 (2017): 158-166.
- [7] Luo, Xin, and Biao Wang. "Structural and elastic properties of LaAlO₃ from first-principles calculations." *Journal of Applied Physics* 104.7 (2008): 073518.
- [8] Luo, X. and Wang, B., 2008. Structural and elastic properties of LaAlO₃ from first-principles calculations. *Journal of Applied Physics*, 104(7), p.073518.
- [9] Mubashir, Shanza, et al. "Pressure induced electronic, optical and thermoelectric properties of cubic BaZrO₃: A first principle calculations." *Optik* 239 (2021): 166694.
- [10] Blanca-Romero, Ariadna, and Rossitza Pentcheva. "Confinement-induced metal-to-insulator transition in strained LaNiO₃/LaAlO₃ superlattices." *Physical Review B* 84.19 (2011): 195450.

- [11] King, P. D. C., et al. "Quasiparticle dynamics and spin–orbital texture of the SrTiO₃ two-dimensional electron gas." *Nature communications* 5.1 (2014): 1-7.
- [12] Blanca-Romero, Ariadna, and Rossitza Pentcheva. "Confinement-induced metal-to-insulator transition in strained LaNiO₃/LaAlO₃ superlattices." *Physical Review B* 84.19 (2011): 195450.
- [13] Min Gyu Ki, J. Phys.: condens.Matter,superconductors, (2012).
- [14] W L Mcmillan Phys. Rev. 167 331 (1968).
- [15] Chein-Lung HUANG, Chil-Chieh CHOU, journal society of Japan, vol 78, aug 2009, 084710
- [16] Walter O Uhoya, Jeffery M Montgomery: J.Phys.: condens matter 23 (2011)122201
- [17] D.S. Jayalakshmi, M. Sundareswari, Indian Journal Phys. 89 (2015), 201-208
- [18] M. Sundareswari and D.S. Jayalakshmi, philosophical magazine, 1478-6435, 2016.
- [19] 1.M. Lifshitz, Sov. Phys. - JETP 11 (1960) 1130-1135
- [20] J.P. Perdew et al., Phys. Rev. Lett. 77 (1966) 386...
- [21] F. Birch, Phys. Rev. 71 (1947) 809.
- [22]I.R. Shein, A.L. Ivanovkii, Solid state communication 151 (2011) 1165-1168
- [23] Sefat A.S., Jin R., McGuire M.A, Phys. Rev. Lett., Vol. 101, pp. 117004