
Study of electronic band structure of Perovskite materials

UNDERGRADUATE THESIS

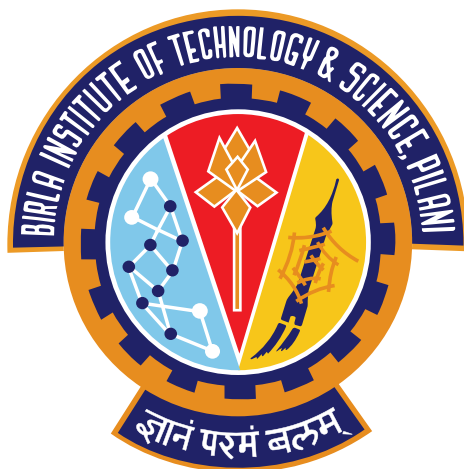
*Submitted in partial fulfillment of the requirements of
BITS F421T Thesis*

By

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December 2023

Declaration of Authorship

I, Vedant TRIPATHI(ID: 2019B5A30582P), declare that this Undergraduate Thesis titled, ‘Study of electronic band structure of Perovskite materials’ and the work presented in it are my own. I confirm that:

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- Where any part of this thesis has previously been submitted for a degree or any other qualification at this University or any other institution, this has been clearly stated.
- Where I have consulted the published work of others, this is always clearly attributed.
- Where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work.
- I have acknowledged all main sources of help.
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This is to certify that the thesis entitled, “*Study of electronic band structure of Perovskite materials*” and submitted by Vedant TRIPATHI ID No. 2019B5A30582P in partial fulfillment of the requirements of BITS F421T Thesis embodies the work done by him under my supervision.

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Abstract

Master of Science (Hons.) Physics

Study of electronic band structure of Perovskite materials

by Vedant TRIPATHI

This study presents a comprehensive exploration of the electronic band structure of perovskite materials, with a specific emphasis on the unique properties of LaGaO_3 . Perovskites, renowned for their diverse and tunable characteristics, are introduced as central subjects for the in-depth analysis of electronic structure. We employ Density Functional Theory as a robust and widely accepted computational framework, with a detailed examination of theoretical principles, including the Kohn-Sham equations. Results encompass structural considerations, electronic band structures elucidating energy dispersion and electronic states, analysis of charge density distribution, and a comprehensive examination of the density of states (DOS). These findings provide valuable insights into the electronic properties of LaGaO_3 and hold significance for its applications in a range of fields, including solid-state electronics and clean energy technologies.

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Abbreviations

DFT **D**ensity **F**unctional **T**heory

DOS **D**ensity **O**f **S**tates

Chapter 1

Introduction

1.1 Perovskite Materials: An Overview

Perovskite materials, named after the mineral perovskite, represent a pivotal paradigm in materials science due to their distinctive crystallographic structure, which embodies corner-sharing octahedra of oxygen ions surrounding positively charged metal cations within a cubic or tetragonal lattice. This atomic arrangement imparts perovskites with remarkable and multifaceted properties that have propelled them into the forefront of materials research. The intrinsic versatility of these materials stems from the intricate interplay between their crystal structure and electronic band characteristics, rendering them indispensable in a multitude of scientific and technological domains.

Perovskite materials are highly malleable in terms of their electronic band structures, enabling them to transition between insulating, metallic, and even superconducting states. This adaptability is fundamental to their widespread utility in advanced electronics, photonics, energy materials, and catalysis. The cornerstone of their scientific relevance lies in the delicate balance between their crystallographic framework and electronic behavior, which underpins their exceptional properties.

Within the pantheon of perovskite materials, LaGaO_3 emerges as a prominent candidate, distinguished by its unique attributes, including high-temperature stability and ionic conductivity. The examination of the electronic band structure of LaGaO_3 assumes particular significance in the quest for a comprehensive understanding of its electronic properties and its potential for applications in areas such as solid oxide fuel cells and sensors. A nuanced comprehension of

the electronic band structure of LaGaO_3 represents an essential component of materials science, promising to unlock innovative solutions and advancements in the fields of energy conversion, electronics, and related technologies. This thesis endeavors to delve into the intricacies of LaGaO_3 's electronic band structure, contributing to the broader discourse on perovskite materials and their role in contemporary materials science.

1.2 Significance of Electronic Band Structure

The electronic band structure of materials is a fundamental concept in condensed matter physics and materials science, offering valuable insights into the behavior of electrons within a crystalline lattice. This topic delves into the significance of investigating the electronic band structure, emphasizing its pivotal role in determining the electrical, optical, and thermal properties of materials.

- **Electronic Band Structure and Material Properties:** The electronic band structure plays a central role in defining the intrinsic properties of a material. For instance, it determines whether a material is an insulator, semiconductor, or conductor, based on the presence or absence of band gaps and the density of states within the energy bands. Additionally, it governs various aspects of a material's behavior, including electrical conductivity, thermal conductivity, and optical absorption.
- **Tailoring Material Performance:** Understanding the electronic band structure offers the potential to engineer materials with desired properties. By manipulating the band structure through doping, alloying, or other means, it becomes possible to tailor a material's performance for specific applications. This level of control has far-reaching implications, ranging from the development of efficient semiconductors for electronics to advanced materials for renewable energy devices.
- **Impact on Technology:** The practical applications of materials, from microelectronics to energy conversion and storage, are intrinsically tied to their electronic band structures. For instance, semiconductors like silicon have revolutionized the electronics industry, while perovskite materials, such as LaGaO_3 , show promise in emerging technologies like solid oxide fuel cells and gas sensors.

Therefore, an in-depth exploration of the electronic band structure of perovskite materials, like LaGaO_3 , is essential for harnessing their potential for technological advancements.

1.3 LaGaO_3 : A Promising Perovskite Material

LaGaO_3 stands out as a particularly promising member, drawing attention for its unique combination of properties. This section delves deeper into why LaGaO_3 has piqued the interest of researchers and its relevance to the study of electronic band structures.

- **High-Temperature Stability:** LaGaO_3 is celebrated for its exceptional stability at elevated temperatures. This property makes it a compelling candidate for applications requiring sustained performance under harsh conditions, such as solid oxide fuel cells, gas sensors, and catalytic processes. The ability to maintain its structural integrity and electrical properties at high temperatures is a testament to its robustness.
- **Ionic Conductivity:** Another defining feature of LaGaO_3 is its ionic conductivity. This property is of paramount importance in the development of solid oxide fuel cells and oxygen sensors, where the material's ability to transport oxygen ions efficiently is pivotal. Understanding the electronic band structure of LaGaO_3 is central to optimizing these applications, as it directly influences the ion migration behavior.
- **Potential Technological Applications:** The remarkable stability and ionic conductivity of LaGaO_3 have positioned it as a valuable component in a range of advanced electronic devices, energy conversion systems, and environmental monitoring tools. Researchers have been drawn to the possibilities of harnessing its properties for clean energy production and efficient gas sensing technologies.

In the subsequent sections of this thesis, we will explore the electronic band structure of LaGaO_3 , providing a comprehensive analysis that underpins the material's suitability for these applications. By deciphering its electronic properties, we aim to unlock the full potential of LaGaO_3 in the realm of materials science and electronic engineering.

Chapter 2

Methodology

2.1 Density Functional Theory

Density Functional Theory (**DFT**) is a quantum mechanical theory used for computationally solving the wave function of very huge systems which consists of multiple atoms and molecules. The theory was developed by Kohn, Hohenberg, Sham and significant efforts to use DFT in computational calculations was made by John. The fact that DFT can be used to solve information about systems as large as DNA complexes and crystals made it largely successful and famous among solid state physicists, computational chemists, material scientists and several others. Today there are multiple programs that use DFT for calculations on complex systems. In this study we use DFT theory for our calculations, and it is impossible to stress the importance and impact of DFT in modern day science.

2.2 Theory

In 1998, Walter Kohn and David John. A. Pople were awarded the Nobel prize in Chemistry for development of Density Functional Theory. Density Functional Theory is a very successful alternative to solving the Schrodinger equation for very complex systems. In order to appreciate just how difficult normally solving a Schrodinger can get, we take the example of a single molecule of NO₂. The Schrodinger equation can be written in its most simplest form as -

$$H\Psi = E\Psi$$

We obviously include the Born-Oppenheimer approximation which approximates the nuclei as stationary particles as they are very heavy. Then we can write the Hamiltonian and Schrodinger equation for NO₂ as follows -

$$\left[\frac{h^2}{2m} \sum_{i=1}^{23} \nabla_i^2 + \sum_{i=1}^{23} V(\mathbf{r}_i) + \sum_{i=1}^{23} \sum_{j < i} U(\mathbf{r}_i, \mathbf{r}_j) \right] \Psi = E\Psi$$

The summation of electrons goes from 1 to 23 since NO₂ has 23 electrons. This is a $23 \times 3 = 69$ dimensional equation. For even larger complexes such as graphene sheets, the number of dimensions ranges in thousands. Clearly solving for the wave function Ψ is going to be a very difficult task. Now if we were to shift our focus from the wave function Ψ to the electron density $n(\mathbf{r})$ which is defined as -

$$n(\mathbf{r}) = 2 \sum_i \Psi_i^*(\mathbf{r}) \Psi_i(\mathbf{r})$$

then the situation looks a lot more feasible since electron density is a function of only 3 parameters while Ψ is a function of 3 N parameters. Therefore we have reduced our problem to 3 dimensions instead of a hundreds and thousands. But we still have to figure out how to relate $n(\mathbf{r})$ to energy of the system and solve for $n(\mathbf{r})$ itself. This is where DFT enters. DFT has 2 main theorems -

- The ground-state energy from Schrodinger's equation is a unique functional of the electron density.
- The electron density that minimizes the energy of the overall functional is the true electron density corresponding to the full solution of the Schrodinger's equation.

These are known as the Hohenberg-Kohn theorems. The first theorem says that there is a direct correspondence between GS energy and electron density. This correspondence is satisfied by a functional, which is an operator that takes a function as an input (in this case $n(\mathbf{r})$) and gives a number as an output(in this case the GS energy). Now we have valid motivation to solve for $n(\mathbf{r})$ instead of the wave function directly. However we have no idea what this functional is that connects $n(\mathbf{r})$ to GS energy. The second theorem tells us that if we knew this "functional" then we could vary the electron density until GS energy is minimum and we would have our desired electron density. We know some terms of this functional from physical insight and we can break into known terms and unknown terms as given in Scholl's book on DFT -

$$E[\Psi_i] = E_{\text{known}}[\Psi_i] + E_{XC}[\Psi_i]$$

where,

$$E_{\text{known}}[\Psi_i] = \frac{\hbar^2}{2m} \sum_i \int \Psi_i^* \nabla^2 \Psi_i d^3r + \int V(\mathbf{r}) n(\mathbf{r}) d^3r + \frac{e^2}{2} \iint \frac{n(\mathbf{r}) n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3r d^3r' + E_{\text{ion}}$$

is the known term contributing to GS energy. The contributions are as follows -

- The first term in E_{known} comes from the kinetic energy of the electron density.
- The 2nd term is from the interaction of the potential $V(\mathbf{r})$ due to the nuclei with the electron density cloud.
- The third term accounts for the interaction of electrons amongst themselves in terms of electron density.
- The last term is the fixed interaction between the nuclei.

The unknown terms denoted by E_{XC} are the exchange correlation terms that we do not know. If we assume that E_{XC} can be obtained in some way, then we are left with the task of solving for the electron density $n(\mathbf{r})$ and plug it in to get the GS energy. But how do we solve for $n(r)$? This problem is solved by the Kohn-Sham equations.

2.3 Kohn-Sham Equations

Kohn-Sham equations are given by -

$$\left[\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) + V_H(\mathbf{r}) + V_{XC}(\mathbf{r}) \right] \Psi_i(\mathbf{r}) = \epsilon_i \Psi_i(\mathbf{r})$$

These equations are used to obtain single electron wave functions that can be then used to obtain the electron density. These equations are basically single electron Schrodinger equations that have the following potentials -

- $V(\mathbf{r})$ is the usual Coulomb potential of interaction between the electron and nuclei.
- $V_H(\mathbf{r})$ is known as the Hartree potential and is given by -

$$V_H(\mathbf{r}) = e^2 \int \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3r'$$

This potential accounts for the interaction between the electron and the electron density cloud. It has a faulty contribution from self interaction of the electron, but it is taken care of in the unknown term.

- $V_{XC}(\mathbf{r})$ is the exchange and correlation effect potential. This potential can be defined appropriately and plugged in the equation.

Notice that the Kohn-Sham equations need the electron density to define the potentials. This means that we have to solve these equations using iteration. To solve for the electron density $n(\mathbf{r})$ we need the single electron wave functions $\Psi_i(\mathbf{r})$, but to determine the single electron wave functions using Kohn-Sham equations, we need the electron density. Therefore we iteratively perform the following steps -

- Start with an initial trial electron density, $n(\mathbf{r})$.
- Then we solve for single particle wave functions $\Psi_i(\mathbf{r})$ for this trial electron density using the Kohn-Sham equations.
- Now we calculate the electron density using the single electron wave functions obtained in the last step. This is done by the usual expression -

$$n(\mathbf{r}) = 2 \sum_i \Psi_i^*(\mathbf{r}) \Psi_i(\mathbf{r})$$

- Now that we have a first order solution for $n(\mathbf{r})$, we can plug it back into the Kohn-Sham equations and repeat steps 1 to 3 repeatedly until we find a satisfactory convergence criteria.

This means that we now have a system of self-consistent equations which can be solved iteratively to determine the electron density $n(\mathbf{r})$ and consequently the GS energy.

Chapter 3

Results

3.1 Computational Details

The computational process involves a series of critical steps to understand the electronic properties of materials. The foundational components are the input files, including the POSCAR, POTCAR, KPOINTS, and INCAR. The POSCAR file encapsulates the structural information, including the unit cell parameters, atomic positions, and the total number of atoms while the POTCAR file provides the pseudopotentials used for efficient electron-electron interaction approximations. The KPOINTS file defines the k-point grid for the Brillouin zone sampling. Finally, the INCAR file allows for detailed control over the electronic structure calculations, enabling the configuration of various parameters and convergence criteria.

Once the input files are prepared, VASPkit is employed for post-processing the VASP output data. VASPkit is a python based tool that helps to extract useful quantities from VASP data. VASPkit facilitates the extraction of essential electronic structure information, specifically the band structure and DOS. The band structure reveals energy band diagrams, while the DOS showcases the density of electronic states across different energy levels. These results are then visualized using VESTA software to provide a clear representation of the material's electronic properties, enabling an in-depth analysis of parameters such as band gaps and electronic states.

VESTA is pivotal in material science, offering an intuitive platform for visualizing crystal structures and charge densities. It enables 3D rendering of complex structures, aiding in understanding atomic relationships and electron localization. VESTA's capabilities for analyzing electronic properties derived from DFT simulations provide valuable insights into material

behavior at the atomic level, making it an essential tool for interpreting crystallographic and electronic data.

3.2 Structure

LaGaO_3 adopts a cubic perovskite crystal structure, which is characterized by a three-dimensional network of corner-sharing oxygen octahedra. This cubic symmetry is one of the hallmarks of perovskite structures and results in several remarkable properties, including structural stability at high temperatures.

In the perovskite structure, LaGaO_3 conforms to the general formula ABO_3 . In this case, "A" represents the larger lanthanum (La) cation, which occupies the center of the unit cell, and "B" signifies the smaller gallium (Ga) cation, which resides at the corners of the octahedra. The oxygen ions (O) fill the gaps, forming the oxygen octahedra.

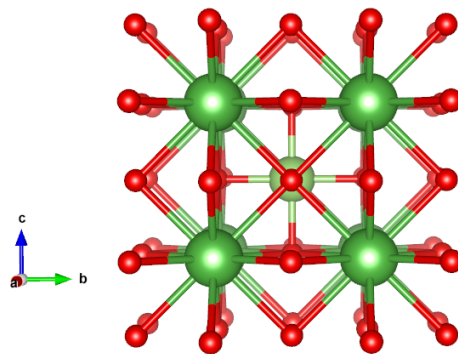
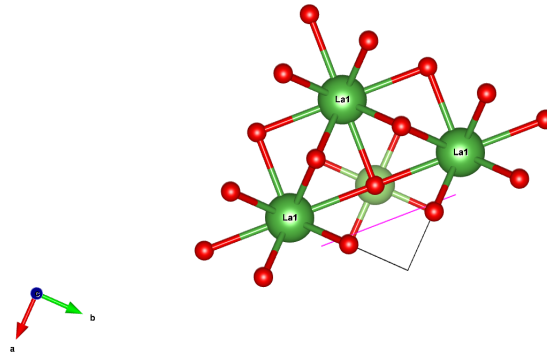
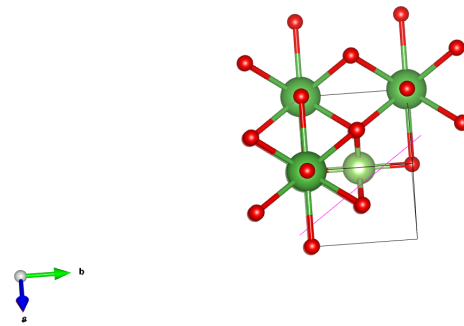


FIGURE 3.1: LaGaO_3 cell structure

On cutting the above structure using the $[111]$ and $[110]$ planes, we get the following results:

FIGURE 3.2: $LaGaO_3$ sliced by 110 planeFIGURE 3.3: $LaGaO_3$ sliced by 111 plane

3.3 Band Structure

Characteristic Parameter	Value of Parameter
Band Gap	3.0893
Fermi Energy	5.7404
Valence Band Maximum (VBM)	5.6102
Conduction Band Minimum(CBM)	8.6995

TABLE 3.1: Electronic Band Structure Characteristics

$LaGaO_3$ features a wide band gap in its electronic band structure, making it an insulating material. The presence of a significant band gap means that there is a clear separation between the valence and conduction bands, and $LaGaO_3$ does not readily conduct electricity under normal conditions. This insulating property is valuable in various applications, such as in solid oxide fuel cells (SOFCs), where $LaGaO_3$ serves as an electrolyte material.

LaGaO_3 exhibits an indirect band gap because its valence band maximum and conduction band minimum are located at different k-points in the Brillouin zone. This indirect band gap characteristic has implications for its optical properties, making it less efficient for applications where direct band gap materials are preferred, such as in certain semiconductor lasers or light-emitting diodes. However, LaGaO_3 's indirect band gap is not necessarily a drawback, as it has other valuable properties, like ionic conductivity.

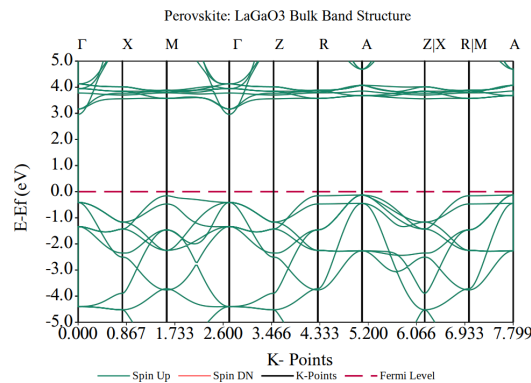
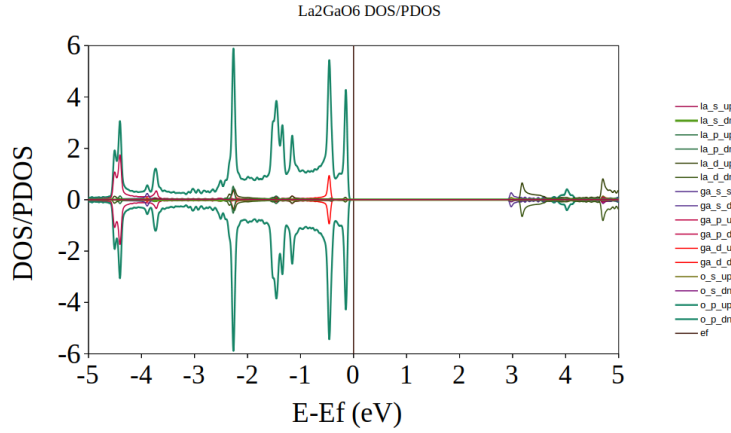


FIGURE 3.4: LaGaO_3 band structure

3.4 Density of States (DOS)

The DOS of LaGaO_3 reflects its wide band gap, which is characteristic of an insulating material. In the DOS plot, there is a clear energy gap between the valence band and the conduction band. This gap signifies that LaGaO_3 does not readily conduct electricity under normal conditions and is an insulator.

A prominent peak is observed near the valence band maximum. This peak corresponds to the density of electronic states in the valence band, which are the states occupied by electrons at lower energy levels. The conduction band appears as a separate region with few electronic states. This low density of states in the conduction band indicates that there are relatively few available energy states for electrons to transition into.

FIGURE 3.5: LaGaO_3 DOS

3.5 Charge Density

The charge density of LaGaO_3 is characterized by the strong ionic bonds that exist between the constituent atoms. Lanthanum (La), Gallium (Ga), and Oxygen (O) atoms have distinct electronegativities, resulting in a transfer of electrons from La and Ga to the oxygen ions. This transfer of charge creates a characteristic charge density distribution, with oxygen ions carrying a negative charge and La and Ga ions carrying positive charges.

The charge density map reveals the arrangement of oxygen ions surrounding La and Ga cations. In LaGaO_3 , the oxygen ions form octahedra around the metal cations, contributing to the material's perovskite crystal structure. The charge density within these octahedra is uneven, reflecting the ionic nature of the La-O and Ga-O bonds. The charge density reveals electron localization primarily around the oxygen ions, leading to insulating properties, as the electrons are bound to the ions.

As we examine the cross-sectional charge density using the 111 plane, we first see that charge is accumulated around the three O ions.

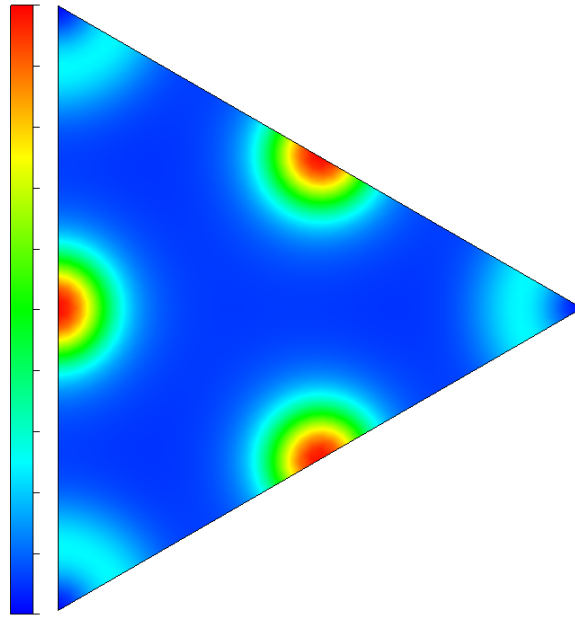


FIGURE 3.6: LaGaO_3 O charge density

As the plane moves further, we cross the O atoms and see that there is no charge density there.

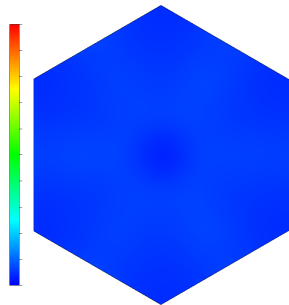


FIGURE 3.7: LaGaO_3 no charge density

Moving forward leads to the formation of another three O atoms as charge centers.

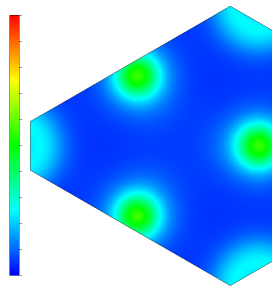


FIGURE 3.8: $LaGaO_3$ partial O charge density

As we begin to exit the cell, we see the charge density of the La atom.

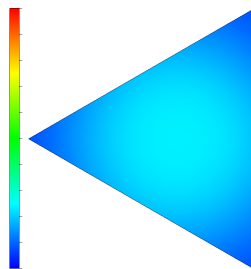


FIGURE 3.9: $LaGaO_3$ La charge density

If we cut along $[001]$ plane, we get a different picture. First we see La atoms charge density forming at 0.014524 distance from origin.

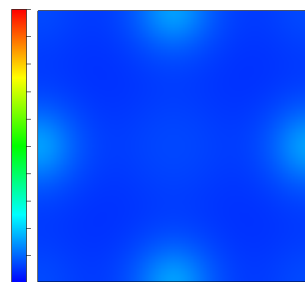


FIGURE 3.10: $LaGaO_3$ charge density at 0.014524

Then we see La atoms charge density around 0.063192 distance from origin.

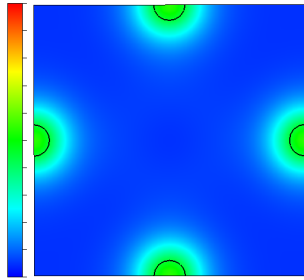


FIGURE 3.11: $LaGaO_3$ charge density at 0.063192

La atoms are at max charge density around 0.081937 distance from origin.

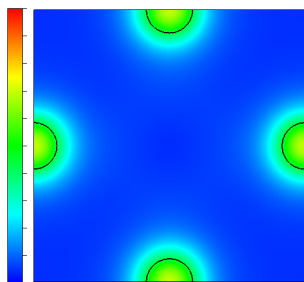


FIGURE 3.12: $LaGaO_3$ charge density at 0.081937

As we move forward, O atoms start to appear around 0.1175 distance from origin.

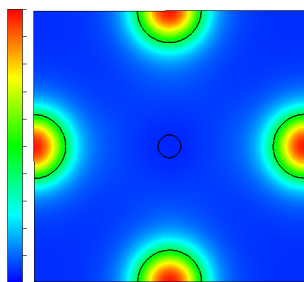


FIGURE 3.13: $LaGaO_3$ charge density at 0.1175

O atoms charge density peak around 0.11967 distance from origin.

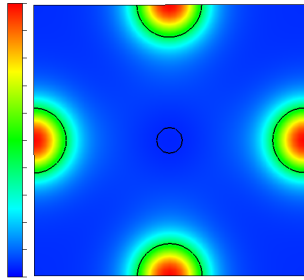


FIGURE 3.14: LaGaO_3 charge density at 0.11967

Near the middle of the cell we also see the density of Ga atom.

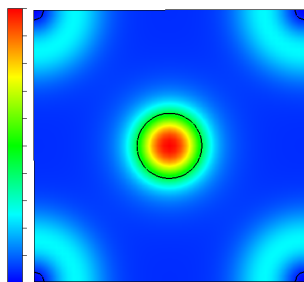


FIGURE 3.15: LaGaO_3 Ga charge density at 0.11967

Chapter 4

Conclusion

In this study, we have embarked on a comprehensive exploration of the electronic band structure of perovskite materials, with LaGaO_3 serving as a notable representative. The intrinsic versatility of perovskites has fueled their significance in materials science, and our investigation underscores the profound influence of electronic band structures on their behavior and potential applications.

The theoretical foundation, rooted in Density Functional Theory (DFT), provided a robust framework for our analysis. The theoretical principles, including the Kohn-Sham equations, guided our approach, facilitating a deeper understanding of the electronic properties of LaGaO_3 .

Our results offer an array of insights into LaGaO_3 's electronic behavior:

- **Structural Insights:** Structural analysis showcased LaGaO_3 's cubic perovskite crystal structure, characterized by oxygen octahedral arrangement. It exhibits insulating behavior owing to a wide band gap, despite challenges in optoelectronic interactions due to its indirect band gap nature.
- **Charge Density Distribution:** Revealed strong ionic bonding within LaGaO_3 , highlighting electron localization around oxygen ions, contributing significantly to its insulating properties.
- **Density of States (DOS):** Comprehensive analysis of the DOS, revealing the distribution of electronic states across energy levels and providing crucial insights into electronic behavior.

- **Implications and Applications:** Findings hold significance for various applications, including solid-state electronics, dielectrics, and clean energy technologies, owing to the insights gained into the electronic properties of LaGaO_3 .

As we conclude, it is evident that the in-depth investigation of electronic band structures and their influence on perovskite materials, exemplified by LaGaO_3 , offers promising avenues for further exploration. The insights gained from this study are pertinent to a broad spectrum of applications, ranging from solid-state electronics to clean energy technologies.

Chapter 5

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