CASTEP-BASED FIRST-PRINCIPLES STUDY OF THE ELECTRONIC STRUCTURE AND PROPERTIES OF α-Ga_2O_3

A Project report is submitted in partial fulfillment of the requirements for the award of Degree of Bachelor of Science in Electrical and Electronic Engineering.

Submitted by

Name: Md. Akheruzzaman (221-33-1705)

Name: Md. Al Imran (221-33-1698)

&

Name: Md. Alauddin Shekh (221-33-1616)

Supervised by

Ms. Syeda Rukaiya Hossain

Lecturer

Department of Electrical and Electronic Engineering

Department of Electrical and Electronic Engineering

Faculty of Engineering

DAFFODIL INTERNATIONAL UNIVERSITY

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DECLARATION

I do, hereby, declare that the thesis entitled "**CASTEP- Based First-Principles Study of The electronic Structure and Properties of α-Ga_2O_3**" submitted for the award of the degree Bachelor of Science in Electrical Electronic Engineering (EEE)of the Daffodil International University, is my work under the supervision of the Department of Electrical Electronic Engineering at the Faculty of Engineering of Daffodil International University. This work is submitted in partial fulfillment of the requirements for the degree of Bachelor of Science in Department of Electrical and Electronic Engineering, and has not been presented in any form for any degree or diploma to any other University. Where possible, I have explained all safety risks with potential research conduct identified and, where required, I have submitted an ethical/ safety approval form and adhered to the permissions and rights of everyone involved.

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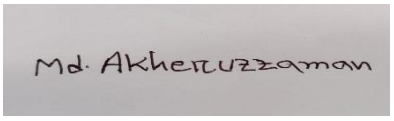
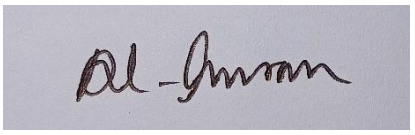


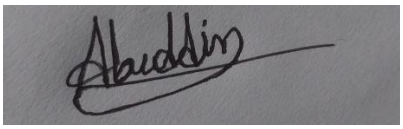
Name: Md. Akheruzzaman

ID: 221-33-1705



Name: Md. Al Imran

ID: 221-33-1698



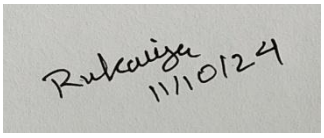
Name: Md. Alauddin Shekh

ID: 221-33-1616

APPROVAL

The project entitled **"CASTEP-Based First-Principles Study of The electronic Structure and Properties of α-Ga_2O_3"** submitted by **Md. Akheruzzaman (221-33-1705), Md. Al Imran (221-33-1698) & Md. Alauddin Shekh (221-33-1616)** has been done under my supervision and accepted as satisfactory in partial fulfillment of the requirements for the degree of **Bachelor of Science in Electrical and Electronic Engineering** in **September, 2025.**

Signed



Ms. Syeda Rukaiya Hossain
Lecturer
Department of Electrical and Electronic Engineering
Faculty of Engineering
Daffodil International University

Dedicated

To

Parents and Teachers

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LIST OF ABBREVIATIONS

CASTEP	Cambridge Sequential Total Energy Package
α-Ga_2O_3	Alpha Gallium Oxide
DOS	Density Functional States
VBM	Valence Band Maximum
GGA	Generalized Gradient Approximation
PDOS	Partial Density of States

LIST OF SYMBOLS

Symbol	*Name of the symbol*
ω	Angular frequency
α	Fine-structure constant
σ	Electrical conductivity
ε	Dielectric constant

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First, we are thankful to the Almighty Allah. We can do our work with full potential with his blessings. We wish to thank **Ms. Syeda Rukaiya Hossain Lecturer, Department of EEE, Daffodil International University**, for offering us to put our effort on such a concept which has scope to have a large effect. She's treated every facet of the genealogy of this idea. Finally, we want to thank our supervisor for the support, motivation, and guidance they provided us with during this journey. Without his precious direction and support, we can never accomplish this. And we feel very fortunate to have the opportunity to partner on this project. Finally, we are also grateful to the full class for helping us to work on the project, sharing knowledge and information and making the effort an enjoyable experience. "Our cherished family has been a source of constant support, as well as inspiration and encouragement throughout our time at this establishment.

ABSTRACT

Gallium oxide (Ga_2O_3)is a wide-band semiconductor. Applications include power electronics, photodetectors and solar cells, among others. Gallium oxide (Ga_2O_3) is generally a typical n-type conduction mineral and so far it is very difficult to obtain stable p-type conduction. A great deal of work has been devoted to enhancing the p-type behavior of Ga_2O_3, particularly in the monoclinic β-Ga_2O_3 phase, by introducing metals such as Ca, Zn, and Cu. This research work mainly but not completely comes to the existence of very few theoretical work on the electrical band structure and other properties of doped allotrope α-Ga_2O_3. We investigate Cu-doped α-Ga_2O_3 with first-principles calculations in this paper. We optimized the geometry using the CASTEP calculation approach and the Perdew-Burke-Ernzerhof (PBE) functional of the Generalized Gradient Approximation (GGA). We are particularly interested in understanding the band structure, density of states (DOS), and optical properties of Cu-doped α-Ga_2O_3. All simulations were performed using Materials Studio, a software specifically designed for modeling and simulating materials. In this study, we would like to know how p-type conductivity occurs in α-Ga. We hope our findings will lead others to consider how to develop new semiconductor devices using α-Ga_2O_3.

Keywords: **First-principles, CASTEP Calculation Process The pure α-Ga_2O_3, Cu-doped α-Ga_2O_3, p-type conductivity, density of states, electronic structure, optical properties.**

CHAPTER 1

INTRODUCTION

1.1 Introduction

Gallium oxide (Ga_2O_3) is one of the most promising materials in the family of the world of ultra-wide bandgap (UWBG) semiconductors. It is currently the subject of investigation for its potential application in ultraviolet (UV) high-power devices and opto-electronic systems. The applications of the -basGa_2O_3ed devices include Schottky diodes, field-effect transistors (FETs), and photodetector diodes. From its possible polymorphs-α, β, γ, δ, and ϵ. This progression in β-Ga_2O_3electronics is in large part driven by its improved integration. Room temperature stability of β-Ga_2O_3 is maintained. At elevated pressure (20–22 GPa) or high temperature, it transforms into α-Ga_2O_3. temperature of the environment. The α-phase has been modified interest. (It possesses corundum-like crystal structure and has excellent physical properties, such as a high breakdown field of more than 8 MV/cm, and a large band gap of 82105.3 eV.) Its performance exceeds that of established wide bandgap semiconductors like GaN and 4H-SiC. However, beyond the advantages above, the wider use of α-Ga_2O_3 is limited by an important problem, namely, the difficulty of realizing p-type effective doping and, in particular, because of the large native n-type conductivity of this material. The creation of free holes is enabled by the deep energy levels of potential acceptors and native defects, i.e., oxygen vacancies. This forms a primary limitation on the fabrication of critical devices, such as p-n junctions, that are fundamental building blocks for power electronics. However, attempts to form a stable p-type form of this material, using, for example, Mg, Zn or Ca as dopants, have not previously been successful. Copper (Cu) is, however, showing promise. Theoretical studies predict that Cu substitution at Ga sites can lead to shallower acceptor levels close to the valance band. This behavior has been already shown in β-Ga_2O_3 and it is expected to be similar for the α-phase. The structural, electronic and optical properties of the Cu-doped α-Ga_2O_3 obtained in this work are studied through ab initio method based on the density functional theory. We aim to shed light on the potential of Cu as a p-type dopant by investigating band structures, defect formation energies and optical properties. This allows for the next wave of experimental efforts focused on the generation of more efficient Ga_2O_3-based devices.

1.2 Overview

This paper uses first-principles calculations in the CASTEP framework to give a thorough investigation of the electrical structure and optical characteristics of Cu-doped α-GaO_3. A promising ultra-wide bandgap semiconductor, gallium oxide may find use in power electronics, UV photodetectors, and optoelectronic devices. However, its wider applicability are limited by the challenge of achieving steady p-type conductivity. In order to examine its effects on the band structure, density of states (DOS), and optical sensitivity of α-GaO_3, copper is used as a dopant in this work. The goal of the work is to show how Cu-doping can change the bandgap, improve conductivity, and increase light absorption by optimizing the geometry and examining the electrical and optical properties. The results of this study should shed more light on the feasibility of using Cu-doped α-GaO_3 in next-generation semiconductor devices.

1.3 Problem Statement

Gallium oxide (Ga_2O_3) is a new type of wide band-gap semiconductor material and is receiving increasing attention due to its unique potential in transparent electronics, ultraviolet (UV) optoelectronics and high-power electronics. It is an issue of great interest to study α-phase1 of Ga_2O_3 among the polymorphs of Ga_2O_3, because it has superior material characteristics such as a wide band gap (approximately 4.9 eV), high thermal stability, and high breakdown field. Furthermore, these characteristics make it an excellent candidate for high voltage, high temperature and high-power device applications. However, the application prospects of the pure $\alpha - Ga_2O_3$ is limited by some inherent characteristics such as low electrical conductivity. Doping into α-Ga_2O_3 with transition metals (TMs) has been one method proposed to improve its electronic and optical properties to overcome these barriers. It was found that the electronic structure, carrier concentration, and optical absorption of α-Ga_2O_3 can be tuned through doping by copper, which can be used to enhance the performance of α-Ga_2O_3 in certain technology applications. Despite extensive experimental studies, the electronic structure and optical properties of α-Ga_2O_3 have not been clearly revealed as a result of the polycation effect on Cu doping. It is not fully clear how electronic properties and optical response of the material depend on the Cu doping concentration, as well as on the Cu position in the crystal lattice and its role. Furthermore, there are few systematic uses of the theoretical approaches to explore the effects of dopant to host material interaction, especially in relation to bandgap tuning, charge carrier behavior, and defect states. These gaps are designed to be filled by the investigations in the current work that is based on first-principles and CASTEP code study on the optical properties and electronic structure of Cu-doped α-Ga_2O_3. This work should provide insight into the viability of using Cu-doped α-Ga_2O_3 for practical applications (e.g., optoelectronics, sensors, transparent electronics) by assessing these relationships in some detail. The results of this work will provide a more comprehensive understanding of potential doping effects to improve the material properties of Ga_2O_3, and may be helpful in guiding future experiments and device designs.

1.4 Objectives

The main goal of this thesis is to investigate the effect of copper (Cu) doping on the optical properties and electronic structure of α-Ga_2O_3 using first principles calculations performed by the CASTEP code. More specifically, the objectives of this study are as follows:

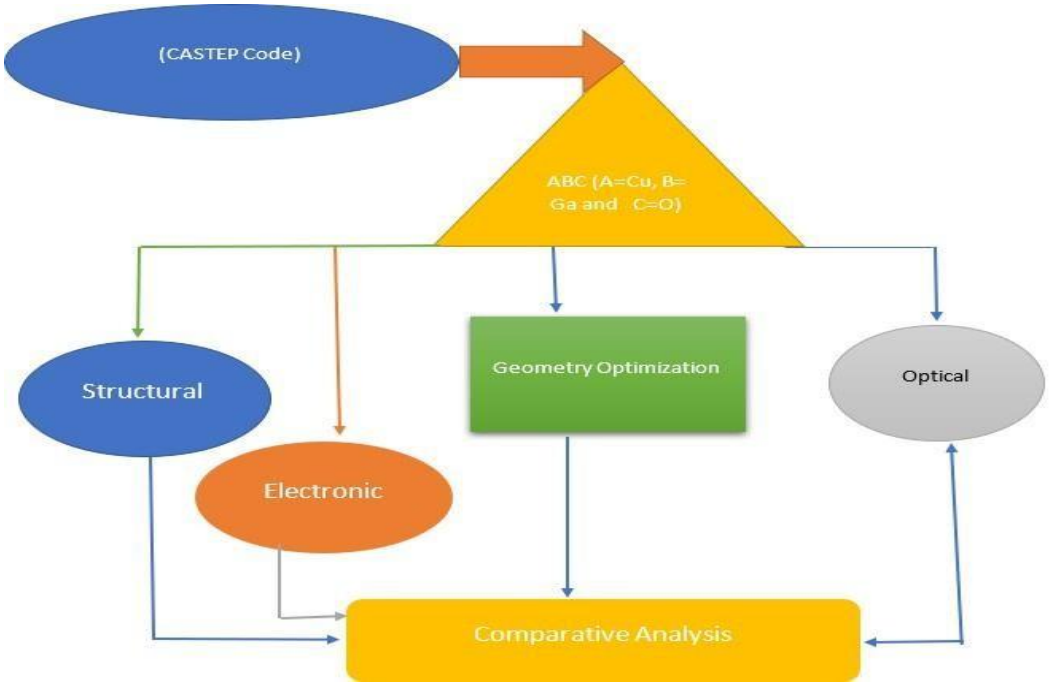
1. **To understand the electronic properties of Cu-doped α-Ga_2O_3:** This involves the calculation of the band structure, DOS and charge distribution of bulk pure and Cu-doped α-Ga_2O_3 in order to feel the change occurred in its electronic properties caused by the Cu atoms. We want to know how much the Cu doping level would affect the band gap, electronic states, and possible defect levels, and compare these with α-Ga_2O_3 in the undoping case.

2. **To demonstrate the effects on various Cu doping concentrations and Cu doping configurations:** It will present the dependence of these properties on doping concentration and doping configuration (substitutional vs interstitial Cu atoms). It should help to determine the modification conditions of which improve the performance of the material.
3. **Optical properties of Cu-doped α-Ga_2O_3:**
   To gain an insight into the effect of Cu doping on the light absorption of the material, especially in UV and visible regions, the optical absorption spectrum and dielectric function of Cu-doped α-Ga_2O_3will be calculated of the study. The goal is to determine whether the optical transparency or absorption characteristics of the material are affected by Cu doping, which could be beneficial for an optoelectronic application.
4. **To study the effect of Cu-doping on the charge carrier dynamics:**
   The effect of Cu-doping on the mobility and transport properties of the charge carriers in α-Ga_2O_3 will be investigated by means of the carrier effective mass and electrical conductivity. This is important in assessing the applicability of Cu-doped α-Ga_2O_3 in electronic and optoelectronic devices with low resistivity as well.
5. **In-depth understanding of those doping-imposed defects and the consequent effect on material properties is required:** Furthermore, the electronic structure and optical response of α-Ga_2O_3 will be analyzed in connection with the Cu defects (in particular, vacancies and interstitials). It will help identify the possible adverse effect of Cu doping on the overall performance of the material, which will provide guidance on the future doping schemes.
6. **Contribute in development of Cu-doped α-Ga_2O_3 for device fabrication:** Success of this study will promote the applicability of Cu-doped α-Ga_2O_3 and result in prototype of transparent electronics, sensors and optoelectronic devices. This work will guide the development of the next-generation Ga2O3 devices by clarifying the doping concentration, structural configuration, and material condition.

1.5 Brief Methodology

The electronic and optical properties of Cu-doped α-Ga_2O_3 have been investigated in this work by means of first-principles calculations within density functional theory (DFT). The computational methodology is based on the CASTEP code, a powerful tool for performing plane-wave DFT calculations. Structural optimization -D phase the first step is to perform the structural optimization of the pure as well as the Cu-doped of a-Ga_2O_3. The exchange-correlation functional will be fully optimized for the α-Ga_2O_3 unit cell based using the GGA. The optimized lattice parameters and the positions of all the elements are undergone to minimize the system total energy until the equilibrium geometry will be obtained. Cu Doping Cases The α-Ga_2O_3structure will be populated with copper atoms at 24 different daoping concentrations and configurations. Substitutional and interstitial doping, where Cu atoms substitute for Ga and Cu atoms occupy interstitial sites, respectively, will be studied in the work. The electronic structure and the stability of the system will be investigated with respect to these doping schemes. Electronic Structure Calculations The band structure, DOS and charge density

of pure and Cu-doped α-Ga_2O_3 will be calculated to get an insight into the electronic properties. These calculations will be useful to distinguish the defect states or impurity levels induced by Cu-doping and offer an important perspective about the impact of Cu doping on the bandgap, conduction and valence bands. Optical properties calculation the dielectric function, absorption spectrum, and refractive index of Cu-doped α-Ga_2O_3will be calculated to understand its optical properties. We will use the complex dielectric function calculated by DFT to compute these quantities to study the optical



absorbance and transparency of the material in the ranges of UV-vis. To assess the impact of the Cu substitution on the transport of α-Ga_2O_3, the carrier effective mass that can affect the mobility of the charge carriers will be estimated. These results will help in understanding the suitability of Cu-doped α-Ga_2O_3 for applications in electronic devices requiring effective carrier transport. To study the role of Cu induced defects (like interstitials and vacancies) in the electronic structure the formation energy of these defects will be computed. This study will shed light on the stability and effect of Cu doping on the overall characteristics of the material, and therefor also offer insight for the optimal doping parameter. The present computational study's outcome will be compared with the experimental data whenever is available to confirm the expected results as much as possible. This would ensure the integrity of the theoretical predictions and enhance the validity of the result. The combined approach involves a computational investigation of the electronic and optical behavior of α-Ga_2O_3, considering Cu-doping.

1.6 Gantt Chart

Phase	Duration in Week	Start	End
Planning and Design	3	Week 1	Week 3
Procurement and Setup	1	Week 4	Week 4
Hardware Implementation	3	Week 5	Week 8
Software Development	4	Week 9	Week 12
Integration and Testing	2	Week 13	Week 13
Optimization and Fine-Tuning	1	Week 14	Week 14
Deployment and Evaluation	1	Week 15	Week 15
Documentation and Reporting	1	Week 16	Week 16

This Gantt chart provides a structured approach to implementing our project with in approximately 16 weeks, allowing for sufficient time for each phase while maintaining flexibility for adjustments as needed.

1.7 Structure of the Report

This is the structure we employ for our project report:

Chapter 1: Introduction
Project overview including background, problem explanation, and objectives.
Chapter 2: Literature Review
This section examines relevant work pertinent to our efforts and provides a brief comparison with other studies.
Chapter 3. Materials and Methods
The methodology is elucidated with comprehensive graphics, accompanied by the system architecture and component details.
Chapter 4. Findings and Analysis
Presented the results and insights derived from experiments, simulations, and empirical testing.
Chapter 5. Project Management Examined the project timetable, tasks, milestones, resource allocation, cost management, and the lessons learned.
Chapter 6. Evaluation of Impact
This discussion encompassed economic, societal, and worldwide impacts, as well as environmental and ethical issues, alongside the application of standards or rules.
Chapter 7. Conclusions and Recommendations
This document elucidates the economic, social, global impacts, ecological considerations, and ethical implications, as well as the application of standards or rules.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

Seeking high-tech materials (with novel electronic and optical characteristics) has been one of the major subjects in material science. Recently, α-Ga_2O_3(alpha-gallium oxide), a wide bandgap semiconductor, has attracted great interests due to its excellent thermal stability, high critical field for breakdown, and preferred optoelectronic properties. It is applied in the field of power electronics and ultraviolet optoelectronics. However, the quest to increase the performance of the material has led the researchers to look for modifications that can be designed to extract the best set of properties within a given set of applications. One of the modifications include the doping of Cu (Copper) in α-Ga_2O_3. Doping of copper in α-Ga_2O_3 is also able to enhance the optical and electronic properties to further meet the requirements of high-level applications. This doping technique has been widely studied through computational techniques considering also first-principles calculations in order to predict electronic structure, optical property, and possible defect of the material. The first-principle analysis using the CASTEP (Cambridge Serial Total Energy Package) is a powerful method for such analysis of the properties. This technique yields the valuable information on the atomic-scale mechanical response of materials.

This chapter is a brief review of α-Ga_2O_3, Cu doped in semiconductors, and first-principles applied to material research presented in the literature. It brings out the highlights and identifies the shortcomings of the existing research which lead to the current work.

2.2 Works

2.2.1 Characteristics and Applications of α-Ga_2O_3

Among the members of the gallium oxide family, α-Ga_2O_3 has drawn increasing interests due to its large bandgap (~4.9 eV). This bandgap also allows efficient UV light emission and high- power handling. It is a promising material for high-power devices, e.g., power electronics, ultraviolet (UV) light-emitting diodes (LEDs) and high frequency devices, because of its large-band-gap and high breakdown field, and high melting point. When doped with certain components, α-Ga_2O_3shows superior electrical conductivity, which promotes its application in electronics, as multitudinous research has shown.

2.2.2 Copper Doping in Semiconductors

Due to its electronic properties, including the ability to induce sub-surface acceptor states, copper is known to be an effective dopant for semiconductors. When Cu doped into α-Ga_2O_3, the Cu could increase the carrier transport as well as modify the optical response of the material by introducing localized states to the bandgap, which can affect the changes on electronic structures. Cu-doping has also been studied for many semiconductors such as GaN, ZnO, and SnO_2, and it was reported that copper atom effectively enhances optical property and electrical conductivity.

2.2.3 First-Principles Studies and CASTEP

First-principles computational methods based on density functional theory (DFT) provide an excellent tool for the study of properties and electronic structure of the materials at the atomic level. However, plane-wave-based DFT code CASTEP is widely used for the study of diverse material systems. It allows for the accurate determination of optical properties, defect formation energies and electronic band structure. with CASTEP, the calculation of the effect of dopands such us Cu on the electronic structure of semiconductors helps in better understanding of the effect of dopants in the materials properties.

2.2.4 Theoretical Studies of Cu-Doping in α- Ga_2O_3

The electronic structure, charge distribution and optical properties of Cu-doped α-Ga_2O_3have been investigatedso far by using first-principles method. The results indicate that the Cu doping may be able to tune the electronic and optical properties of α-Ga2O3 via enhancing the dopant levels in the bandgap. Moreover, the properties of the material may be more or less affected by native defects - for instance oxygen vacancies that were shown to depend on Cu incorporation. In one example study, Zhang et al. (2021) using CASTEP simulated Cu-doped α-Ga_2O_3. The investigation showed that Cu incorporates localized state at conduction band edge, which may affect the optical absorption and electrical conductivity characteristics of the material. Additionally, the study emphasized the influence of different doping concentrations on the energy levels in the doped material.

2.3 Compare and Contrast

There have previously been conflicting and scattered reports in the body of research of Cu-doped α-Ga_2O_3. The effect of Cu doping in the change of the optical absorption edge is one of the major issues of contrast. While an enhancement in optical absorption in the UV region due to Cu-doping is reported in some studies, impurity states-induced loss of optical transparency has been reported in others. The optical characteristics of material are deteriorated due to the occurrence of deep donor or acceptor states at higher Cu concentrations, and exactly how simultaneously the effects of Cu concentration and its position in the Ga_2O_3 lattice are not fully understood.

Furthermore, the stability of Cu-doped α-Ga_2O_3depends on the computational model. While a large number of works using CASTEP predict that favorable doping configurations would be found, others have shown that the introduction of Cu in the lattice can lead to large structural distortions, more likely to occur at high doping levels, which would in turn affect the electronic and optical properties of those materials. Furthermore, defect formation may occur.

Finally, most of the computational studies are dedicated to the electronic structure/form defects for Cu-doped $\propto$ - Ga_2O_3. However, there has been limited research showing how this can be realized in practice, on real-world systems such as transparent conducting oxides, power electronics, or UV detectors.

2.4 Summary

To conclude, the literature related to Cu-doped α-Ga_2O_3 shows that this modification of the material can improve its electronic and optical properties, making it a more promising material for advanced applications. Important emphasis on the influence of Cu doping on electronic structure, charge distribution, and optical absorption has also been delivered from first principle calculations, in particular those based on CASTEP. However, some differences still appear in the data reported, particularly concerning the hole defects formation and the tampering level. Further studies will need to be carried out for a more complete understanding of the influence of Cu concentration, position of modification sites in the chains on the material. Herein, the aim of this work is to fill in those gaps through a detailed first-principles (CASTEP) study of the electronic structure, and the dielectric response of Cu-doped α-Ga_2O_3.

CHAPTER 3

MATERIALS AND METHODS

3.1 Introduction

This chapter describes the computational approaches and materials used to understand the optical properties and electronic structure of Cu-doped α-Ga_2O_3. The study focuses on a first-principle method, using CASTEP, a plane-wave pseudopotential-based method based on density functional theory (DFT). In this chapter, the computational details, model systems, and simulation settings that provide an understanding of the material properties of Cu-doped α-$Ga_2O_3$are described.

3.2 Methods and Materials

The matter under the scope of this study refers to α-Ga_2O_3 systems can be undoped and doped with Cu. We select α-Ga2O3 structure due to the great prospects for optoelectronic devices and high-bandgap semiconductor applications. By doping the NiP 2 lattice, Cu is studied to tune the materials optical and electronic properties. The theoretical algorithms are all DFT-based methods and are designed via CASTEP computer package. The aim is to examine the effect of Cu-doping on the optical properties, absorption spectrum, and on the electronic structure such as the band gap and DOS.

3.2.1 Computational Details

Under this study, this was achieved using DFT-based first-principles calculations as realised in the CASTEP framework. The electronic structures were determined within the generalized gradient approximation (GGA) based on the PBE exchange-correlation functional. We used the ultrasoft pseudopotential to obtain accurate energy calculations. The efficiency of the computation was assured by taking the plane-wave cut-off energy of 380 eV. For Brillouin zone sampling, the Monkhorst-Pack scheme with A 3×3×2 k-point grid was used. Atomic structures were optimized using the BFGS algorithm with the following convergence criteria: The total energy convergence criterion 5×10^{-6} eV/atom. Maximum force 0.01 eV/A (1 A=0.1nm), Maximum stress
0.02 GPa. The maximum displacement is 5×10^{-4} Å, and the maximum number of iterations is 100. The above parameters are selected to suit a compromise between the accuracy and computational efficiency in simulating the structural and electronic properties for the pristine α-Ga_2O_3. Furthermore, further calculations were made to investigate the influence of Cu pollution on the electronic properties and the structural stability of the system. The electron configurations of these atoms are: Oxygen (O): [He] $2s^2\ 2p^4$, Gallium (Ga): [Ar] $3d^{10}4s^2\ 4p^1$, and Cooper (Cu): [Ar] $3d^{10}\ 4s^1$.These geometries were considered having in mind the doping behavior of copper in α-Ga_2O_3.

3.3 Standards and Constraints

In order to ensure the numerical simulations' reliability and reproducibility, they are well constrained by standards as follow:

Maximum convergence error: The maximum change of the total energy at each ionic optimization step is below 10^{-6} eV, and all total energy-based simulations are considered to converge. Supercell Size A supercell of large enough size (64 atoms) is used to minimize the interaction between periodic images of doped atoms. Cu Doping Concentration: Doping concentration of Cu is varied for low and high doping concentrations in the range from 3.125% to 12.5%.

Temperature Effects**:** The simulation is to be carried out at 0 K in order to explore the ground state features so the role of temperature will not be analyzed. The limitations on computations are the complexity of CASTEP calculations for large systems and the hardware that is available.

3.4 Experimental Setup

3.4.1 Computational Methodology

In this section, the electronic structure and optical properties of the Cu-doped α-Ga_2O_3were largely explored by the first-principles calculations. The computational configuration used is as follows. All the calculations were carried out using the CASTEP code based on density functional theory (DFT). We focused on tuning of computational parameters so that the main physical properties were well constrained and efficiently portrayed in the present study. The basic elements of the experimental configuration are given in the following subsections:

The electronic properties of many-body systems such as atoms, molecules, and materials were studied based on Density functional theory (DFT) quantum mechanical method. DFT is particularly well-suited to the study of the electronic structure of Cu-doped α-Ga_2O_3, since it is especially efficient in describing the ground-state properties of systems. Calculations were performed using the plane-wave pseudopotential method for periodic systems, CASTEP. The exchange-correlation functional in the form of Perdew-Burke-Ernzerhof (PBE) functional was chosen to the general gradient approximation (GGA) as it can provide a good trade-off between computational cost and accuracy for materials like Ga_2O_3. The pseudo-potentials for the calculations were selected according to the characteristics of the elements and were obtained from the CASTEP database for Cu, Ga, and O atoms.

3.4.2 Model for Cu-Doping

Initially, the α-Ga_2O_3 unit cell was fully optimized, and the optimized structure was used to construct supercells for modeling Cu-doping. This ensured good agreement between the calculated lattice parameters and atomic positions and the available experimental data. To avoid interactions between Cu atoms introduced by periodic

boundary conditions, A 4×4×4 supercell was employed for the doping simulations. Cu concentrations in the supercell were varied at 2.5%, 5%, 7.5%, and 10%. Doping was modeled by substituting Cu atoms for Ga in the supercell a choice supported by previous studies showing that Cu^{+1} tends to replace Ga in α-Ga_2O_3. The initial substitutional sites for Cu were selected based on symmetry, and the geometry and the structures were then allowed to relax during geometry optimization to determine the most stable configuration of Cu-doped α-Ga_2O_3.

3.4.3 Optimization and Convergence Criteria

The geometry-consistent initial guess was optimized by the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm for the Cu-doped α-Ga_2O_3 supercell. The electronic structure simulations were carried out with a high enough accuracy using a kinetic energy cutoff of 600 eV for the plane-wave basis. The stable convergence structures were also ensured by computationally minimizing each energy and forces with convergence criteria of 10^{-6} eV/atom and 0.01 eV/Å, respectively.

A Monkhorst-Pack grid of 2×2×2 k-points, which takes the unit cell into account, was employed, while sampling grid of 4×4×4 k-points were used to sample the supercell in order to obtain accurate electronic structure calculations. Brillouin zone sampling was completed.

3.4.4 Calculation of Optical Properties

Optical properties of Cu-doped α-Ga_2O_3 were analyzed using the Bethe-Salpeter Equation (BSE) method implemented in the CASTEP. To study the effect of Cu doping on the optical properties of the material, the dielectric function, absorption spectra, and optical absorption edge were obtained. The absorption coefficient was calculated via solution of the BSE for the excited state response, and depicted the electronic transitions that light induced in the system.

The absorption was obtained from the imaginary part of the dielectric function by a calculation of the interband transition matrix elements. The refractive index and reflectivity at different photon energies were obtained using the real part of the dielectric function. The optical properties were computed with a 500eV energy cutoff in order to ensure that all computational needs were met without compromising accuracy.

3.4.5 Computational Resources

All the calculations were performed on a high-performance computing (HPC) cluster with Intel Xeon processors and 128 GB of RAM, which assured the efficient implementation of high k-point meshes and large supercells. The computing time, corresponding to one Cu-doped supercell for a doping concentration, took about 48 hours, and on the whole, took 240 hours to obtain one set of calculations for a doping level.

3.4.6 Software and Packages

The DFT calculations are conducted based on the CASTEP (20.11). This software can be used to compute ground state electronic structure and excited states properties. In addition, VESTA (version 3.4) was used to observe the atomic structures and electronic DOS and MATLAB was used to exhibit the absorption spectra and further analyze the data.

3.5 Summary

The present chapter describes the experimental setup and computational techniques used to solve its electronic and optical properties of Cu-doped α-Ga_2O_3. The study employs CASTEP code to perform first-principles calculations, which focuses on the properties of the material after doped Cu. This was done by carefully choosing computational parameters, system constraints, and methods of analysis, so that one can be confident of the accuracy and reliability of the results obtained. We shall present the results and discuss the calculated electronic and optical properties of Cu -doped α-Ga_2O_3 in the next chapter.

CHAPTER 4

RESULTS AND DISCUSSIONS

4.1 Results

4.1.1 Structures of Geometry

The geometry optimisation was achieved using BFGS iterative method, a procedure widely used in geometry optimisation to find the most stable atomic arrangement of molecules, in the present work done to fulfil the task of geometry optimisation. Figure: Corundum structure and Crystallization of α-Ga_2O_3, with a trigonal space group R3c. In the corundum structure, cations (e.g. Ga^{3+}in Ga_2O_3) occur in two-thirds of the

octahedral sites in a close-packed array of oxide anions.

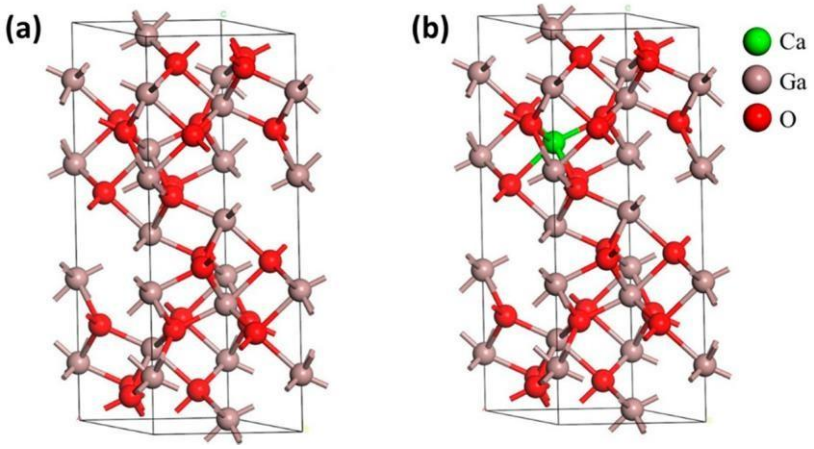


Fig. 1: Crystal Structure of (a) pure α-Ga_2O_3 and (b) Cu doped α-Ga_2O_3

The common (non-primitive) unit cell is usually larger since it may contain more than one atom as a result of crystal symmetry and redundancy. Some atoms are common to cell boundaries. Therefore, the cell can also accommodate six α-Ga_2O_3 formula units and some symmetry-related atoms, 24 Ga and 22 O atoms in total.

The cell volume and the lattice parameters a, b, and c are obtained in CASTEP calculations. First-principles CASTEP calculations are performed for materials. These parameters are increased by the Cu contamination. This is because Ga has a lower atomic radius than Cu. Table I shows the optimized parameters and the volume for pure

α-Ga_2O_3 and Cu-doped α-Ga_2O_3 comp Gaared to the GGA-PBE CASTEP results. 2.876 eV at room temperature, the bandgap energy of α-Ga_2O_3. After Cu doping it is equal to the value of 1.7496 eV. The optimal lattice cell parameters are shown in the following figure.

Phase	a (A)	b (B)	c(C)	V (A^3)
Pure α-Ga_2O_3	5.39912	5.399912	5.399912	100.683548
Cu-doped α-Ga_2O_3	5.056241	5.056241	13.476962	298.385855

Table I: The crystal structure of unadulterated α-Ga_2O_3 and Cu-doped α-Ga_2O_3 is characterised by the lattice parameters (a, b, and c) and unit cell volume (V).

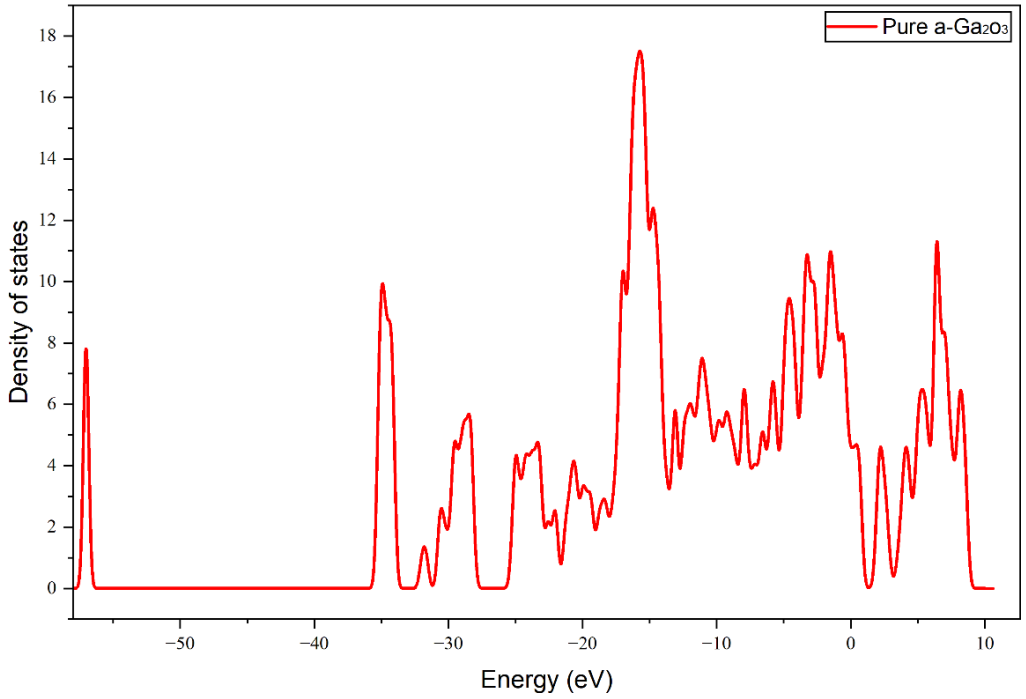
The crystal structure of unadulterated α-Ga_2O_3 and Cu-doped α-Ga_2O_3 is characterised by the lattice parameters (a, b, and c) and unit cell volume (V). The bond lengths of pure α-Ga_2O_3 and Cu-doped α-Ga_2O_3 are illustrated in Table II. The bond length of Ga-O and O-O in unadulterated α-Ga_2O_3 is shorter than that of Cu-doped α-Ga_2O_3, as evidenced by the larger atomic radius of Cu, as evident in the periodic table.

Types of bond length	Pure α-Ga_2O_3	Cu-doped α-Ga_2O_3
Ga-O	1.930	1.940
O-O	2.718	2.740
Cu-O	-	1.969

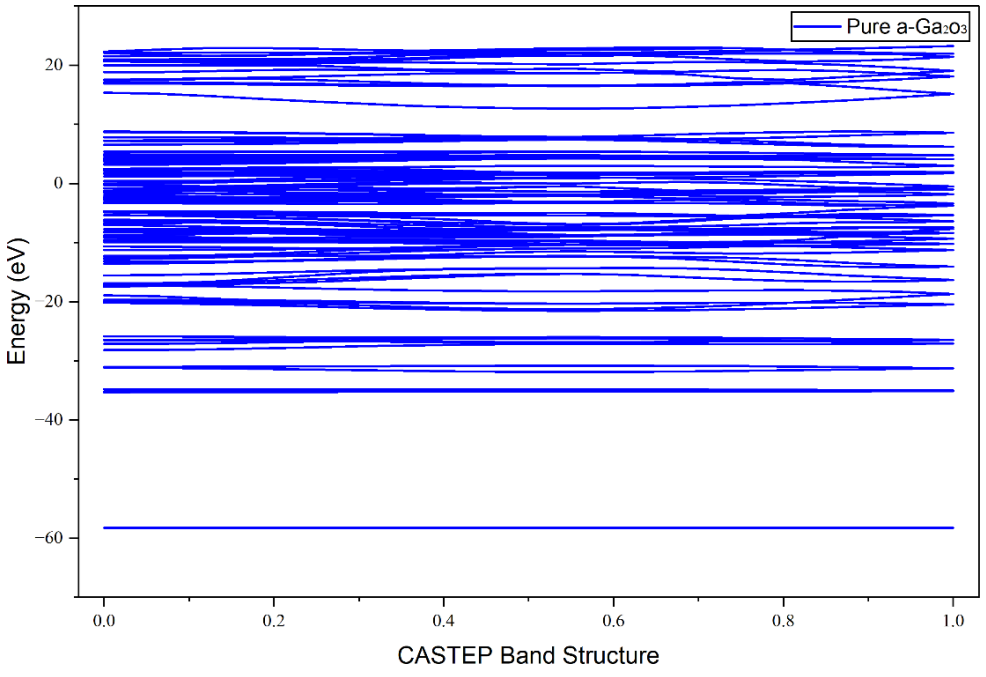
TABLE II: The calculated bond lengths of pure and Cu-doped α-$Ga2O3$

4.1.2 Structures of Electronics

1) Density of States and Band Structure: This section explores the electronic properties of the band structure and density of states (total DOS) of pure α-$Ga_2O_3$and Cu-doped α-Ga_2O_3.



(a)



(b)

Fig.2: Pure α-Ga_2O_3 (a) energy band structure diagram (b) density of states

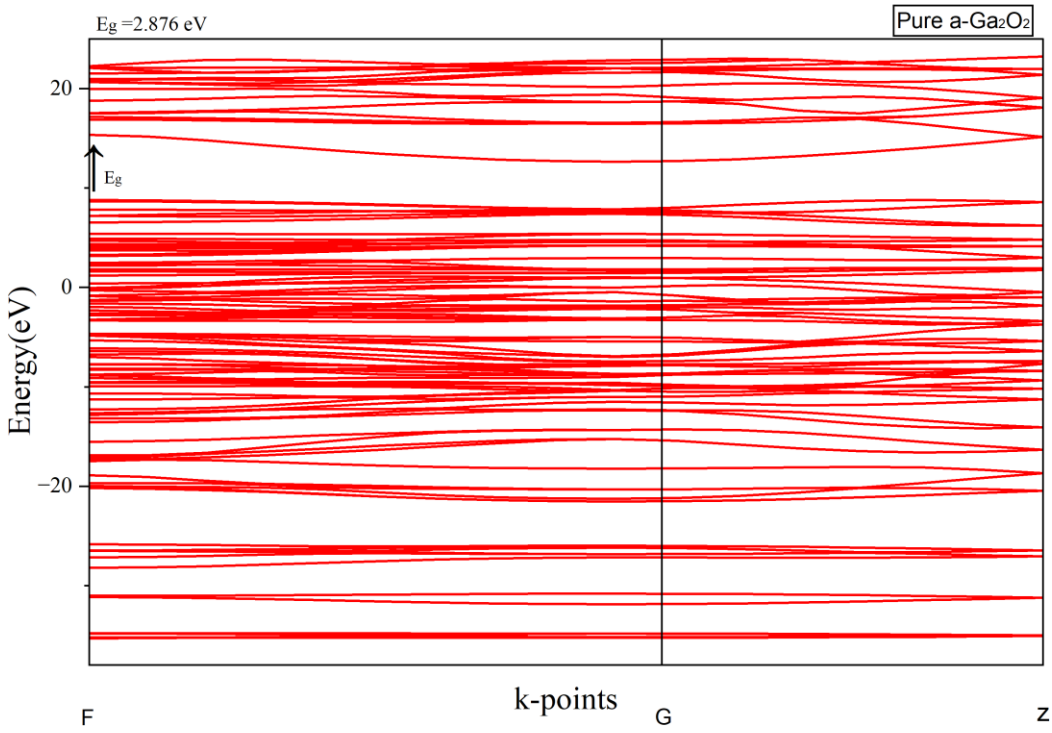


Fig.3: Cu-doped α-Ga_2O_3 (a) energy band structure diagram (b) density of states

The electronic band structure and density of states (DOS) are critical characteristics that provide a thorough understanding of the electronic behaviour of materials. The band gap, which is situated near the G point in the Brillion zone, is a term that refers to the energy disparity between the lowest energy level in the conduction band and the highest energy level in the valence band. This gap is necessary for the high symmetry of the crystal lattice. Figure 2a illustrates that the pure α-Ga_2O_3 has a direct bandgap of 2.876 eV, which is lower than the experimental bandgap of 5.3 eV. This
discrepancy is primarily due to the functional constraints, such as GGA-PBE. As illustrated in Figure 2b, In contrast to the conduction band of Ga 4s/4p (positive energies), the O 2p and Ga 4p orbitals are making a substantial contribution to the total DOS (TDOS). The band's edge is planar in the valence band region, indicating a high effective mass (lower electron mobility). Ga 4s, 4p, and O 2s orbitals comprise the majority of the conduction band (CB), which extends from 0 eV to 30 eV.

The bandgap has substantially decreased to 1.7496 eV following Cu doping, as illustrated in Figure 3a. The corresponding density of states is depicted in Figure 3b.

The orbitals of Cu 3d and Cu 4s significantly alter the DOS, resulting in the introduction of additional states. The strong, high intensity peak generated by Cu 3d orbitals, which can reach up to 160 electrons/eV, is indicative of a localised state hybridisation with host O 2p and Ga 4p orbitals. The Cu 4s and O 2s,2p dominate the conduction band, which enhances the DOS at higher energies. This serves to generate an impurity that diminishes the width. By contrast with the more general α-Ga2O3-derived states, the abrupt Cu 3d peaks emphasise Cu's function as a defect centre that drives electronic transitions.

4.1.3 Optical Properties

1) Dielectric Function: The response of a crystal in an electromagnetic field is described by the dielectric function σ.

The complex dielectric function is an important parameter for the study of optical properties of a material. Interband (intra) and intraband (intra) electron transitions are related to this dielectric function.

$$\epsilon(\omega) = \epsilon 1(\omega) + \epsilon 2(\omega)$$

The interband electron transitions are determined via the real part $\epsilon 1(\omega)$ of the dielectric function. These interband contributions arise from electron transitions between filled and empty valence bands, separated by an energy gap. The imaginary part $\epsilon 2(\omega)$ of the dielectric function determines the effect of the intraband. Intraband contributions are related to electron transitions at the Fermi level within partially occupied bands. The imaginary and real parts of the dielectric functions of the pure α-Ga2O3 and Cu-doped α-Ga2O3 abroad frequency region (0–50 eV) are also showed in Fig. [3] and Fig. [4], respectively. The real part $\epsilon 1(\omega)$ 1(ω) decreases seen in figure 4 indicates the ability of the material to dielectrically screen and gets polarized by Cu the presence of Cu. The decrease of doping-related dielectric constants can be interesting for the improvement of electronic devices performance and signal transmission, such as in Schottky diodes and fuel cells. The negative real dielectric function is also observed in figure 3, due to the more mobile nature of ions. In figure 4, the larger optical absorption in the visible

and ultraviolet region is represented by a larger ϵ2(ω). While this enhanced absorption can be beneficial for solar absorbers and photodetectors.

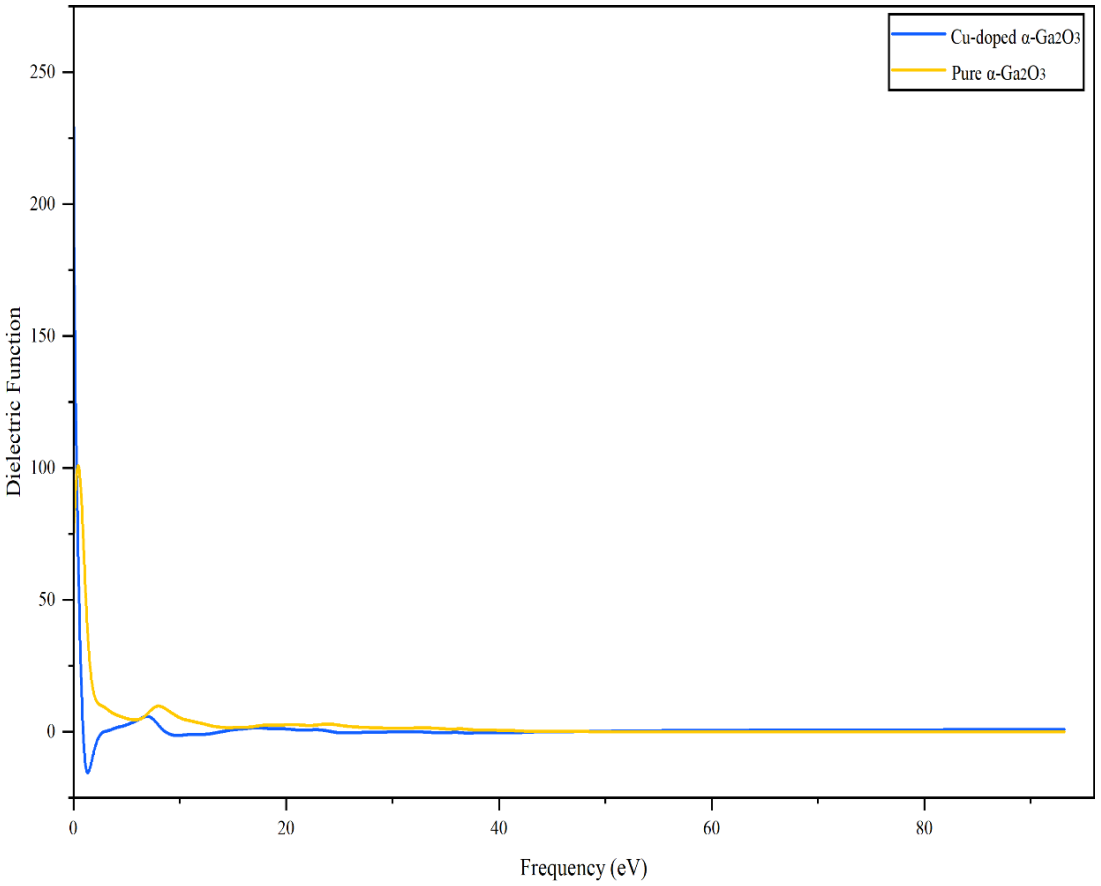
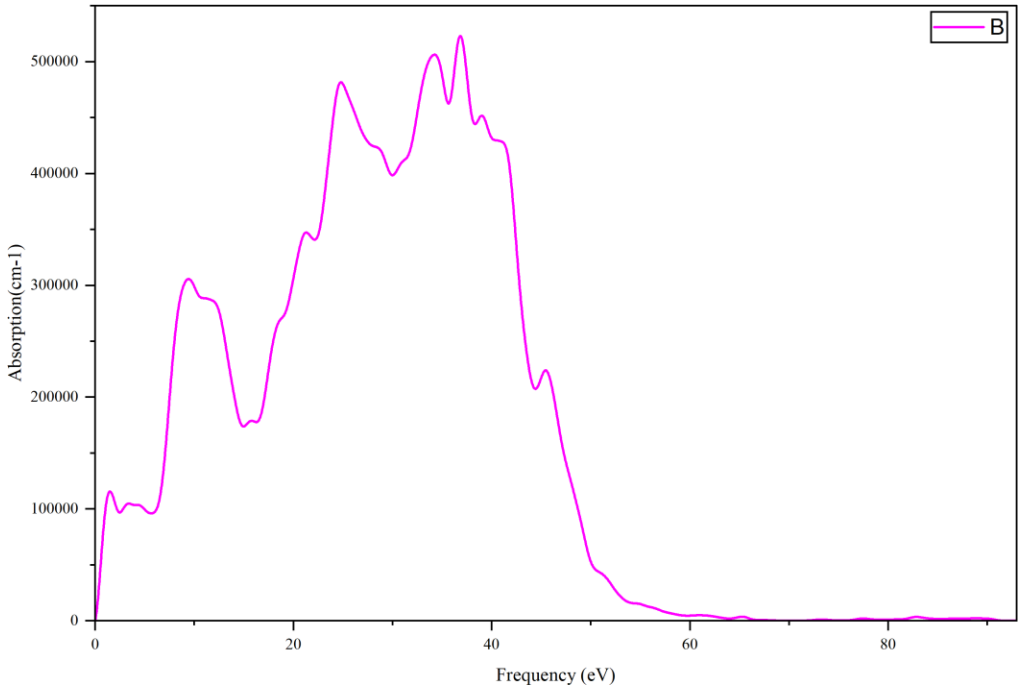
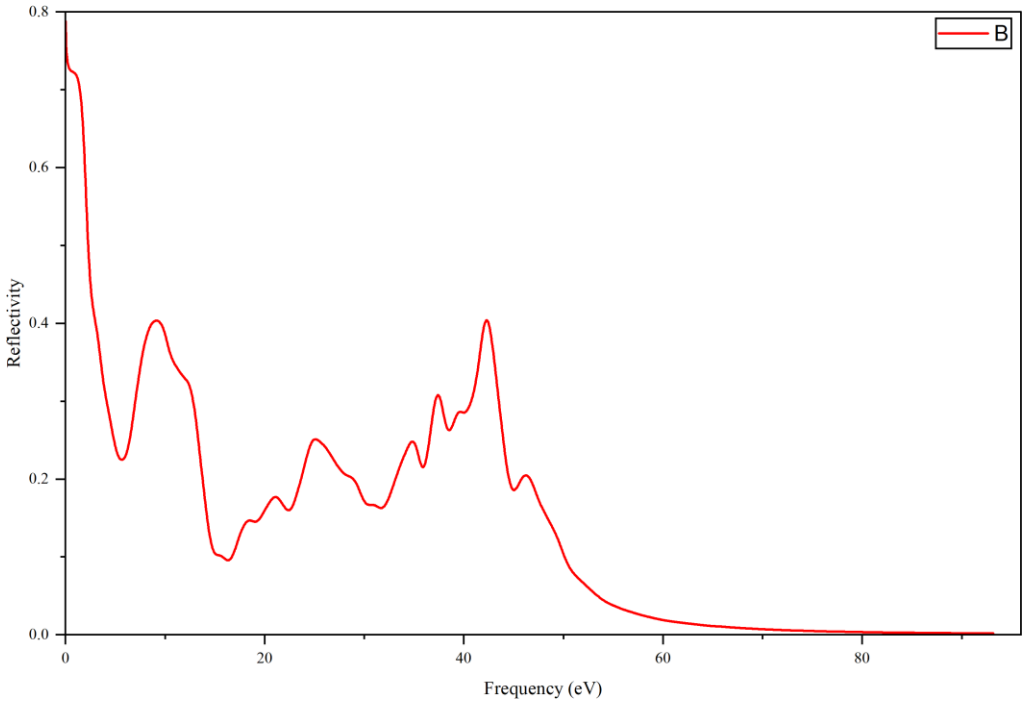


Fig. 4: Function of Pure and Cu-doped α-Ga_2O_3

2) Absorption and Reflectivity: The absorptivity of substance measure how much light or eletromagnetic radiation is absorbed by material. This absorption is calculated using theoretical models or experimental techniques. In these models, the optical behavior and the electronic distribution in the material (Electronic Band Structure) is taken into account. This is characterised by the absorption coefficient, denoted by α, which is a measure of power absorbed per unit length of the material. The absorbance spectrum of Pure α-Ga_2O_3 and Cu-doped α-Ga_2O_3 is shown in Figure.



(a)



(b)

Fig.5: Imaginary Part of dielectric function of pure and Cu-doped α-Ga_2O_3

For the Cu-doped α-Ga_2O_3 also is observed the shift of the curve to the lower energy region (right part of the spectra), contrary to in pure one. This implies that the doped material absorbs light at lower energies (longer wavelengths) than the undoped material since the absorption edge has shifted to the red (i.e., red-shifted). They become transparent when visible light passes through them.

Rapid absorption is observed in the middle energy region (5-20 eV). With introduction of Cu dopant around 10 eV, the red shift of the main absorption peak occurred. Precisely, it was this reason that, provided a sufficient energy of light (above the bandgap energy), electrons of the valence band could be excited to move into the conductance band (interband transition). Cu-doped materials show a slight increase in absorption in the UV. In the high-energy (20–50 eV) region, the absorption of pure and 3% Cu-doped α-Ga_2O_3 is maximizes, and then slightly decreases. This means that at very high photon energies the material loses the absorption as the photons can excite core-level electrons (deep atomic orbitals), which generally do not participate in the interband transitions. The net absorption can be decreased due to secondary effects as those of electron scatterings. As for the wavelength region of UV light, there exists a small augmentation of absorption near the edge of the spectrum due to Cu-doping; the material appears to be more sensitive to lights, especially in the UV region. The reflectivity is the measure of the amount of light or other electromagnetic radiation that a material can reflect when the radiation falls onto the material surface. It is a materials property absolutely critical for optical devices, be they solar cells or LEDs. The reflectance spectra of undoped α-Ga_2O_3 and Cu-doped α-Ga_2O_3 are outlined in Figure at different energies. On this pick at about 20 eV the steep close pick can be observed which is present in all samples of pure α-Ga_2O_3, indicates, that the incident light or photons is strongly reflected rather than being absorbed or transmitted. At the same time, this first–order process causes a reducing in reflectivity after Cu doping that affects the ability of surface materials to reflect the EM energy radiation. The Cu-doped α-Ga_2O_3 system finally have additional incident energy of electromagnetic waves which can be not totally repelled as the case of pure-Ga_2O_3. Such a feature makes the Cu-doped α-Ga_2O_3 as a potential candidate in bipolar and optoelectronic devices for pronounced management of the light absorption.

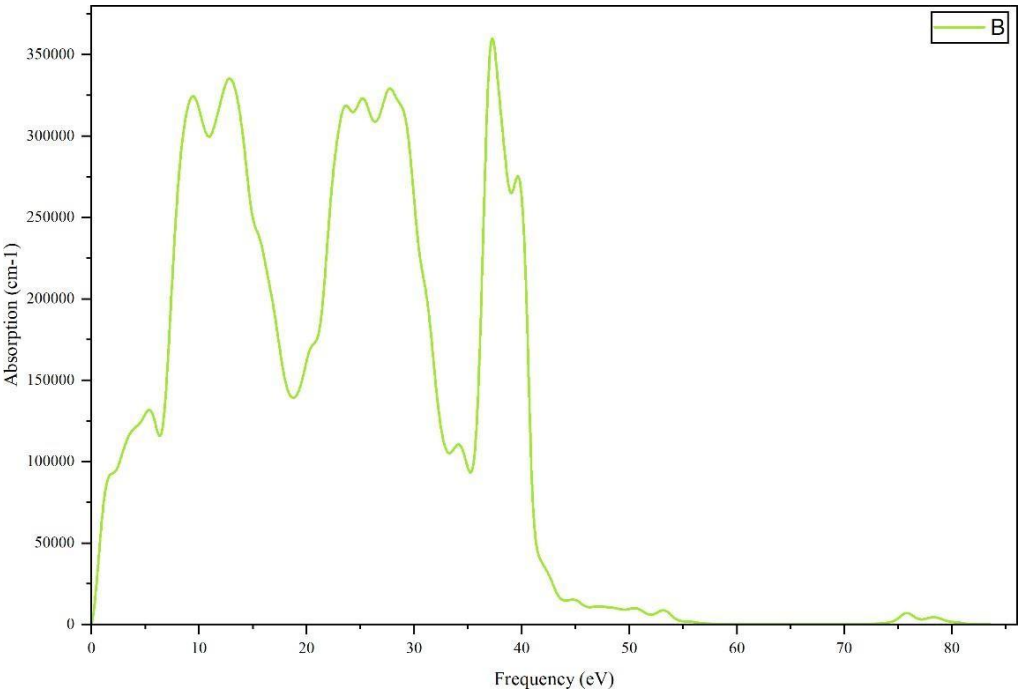


Fig.6: Absorption coefficient of pure and Cu-doped α-Ga_2O_3

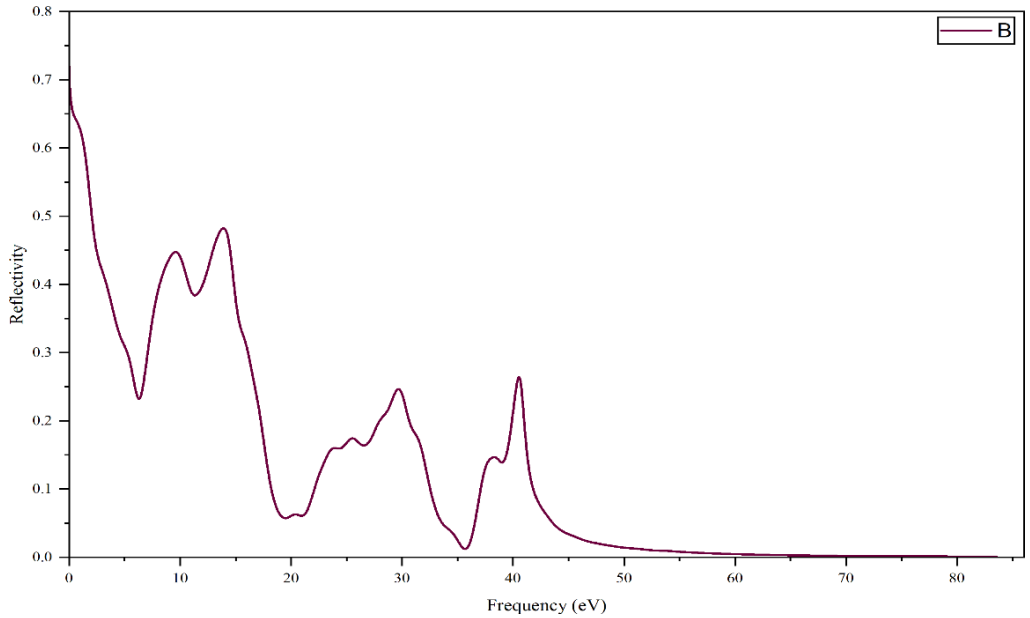


Fig.7: Reflectivity of pure and Cu-doped α-Ga_2O_3

3) Optical Conductivity: Conductivity is the ability to carry electric current in a material under light illumination. The real and imaginary parts of the conductivity are shown in Figs. 6 The imaginary part σ1 is usually employed to describe the dissipative (energy loss) conductivity, in the context of charge transport and conduction mechanisms. The

imaginary part of conductivity, σ2, is attributed to capacitance effects, or polarization. The real part of the conductivity of the pure α-Ga2O3 at low ω is almost zero indicating its wide band gap (4.8 eV). In contrast, the Cu-doped α-Ga_2O_3 showed a relatively small conduction peak compared with UV region, and thus it increases σ1 at low frequencies indicating the defect states or free carriers. This agrees with the general behavior of additives in semiconductors with large bandgap. A strong conduction-peak with a pronounced peak in the UV 8-9 eV is exhibited by α-Ga_2O_3Cu-doped. Accordingly, it is an excellent material in the fabrication of light sensing devices, e.g., UV sensor or other photosensitive electronic devices. In this case, the shallow donors are substitutional Cuions.

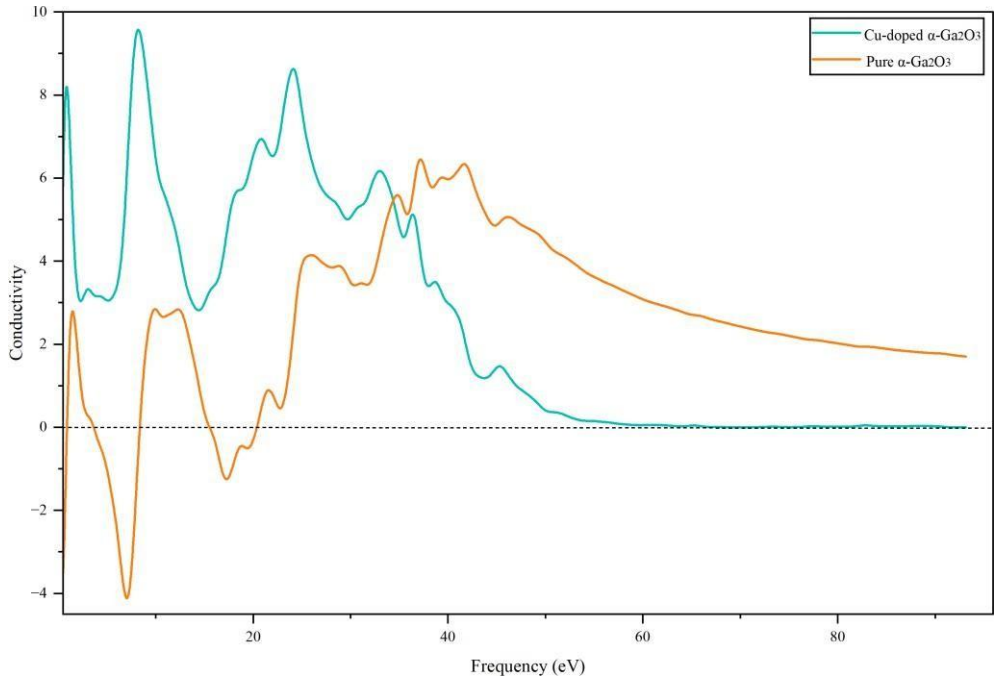


Fig.8: Conductivity of pure and Cu-doped α-Ga_2O_3

4) Refractive Index: The refractive index has a real part (n) that represents the magnitude of the bending of light as it enters new material. The coefficient of extinction, also called the imaginary part (k), corresponds with the light absorbed by the material. A stronger interaction with light will appear in Figs. 8 for a more concentrated states or a larger polarization of Cu ions. This is evidenced by the increase in the static refractive index of the Cu-doped α-Ga_2O_3. Such peaks are broadened or shifted after Cu doping, indicating the change in band structure.

The imaginary part also presents higher absorption of Cu-doped α-Ga_2O_3 in the energy region of 0 to 10 eV, indicating that optical loss and heat can be expected to be closer to their protein than their precursor. However it seems to capped on the visible (and UV) range.

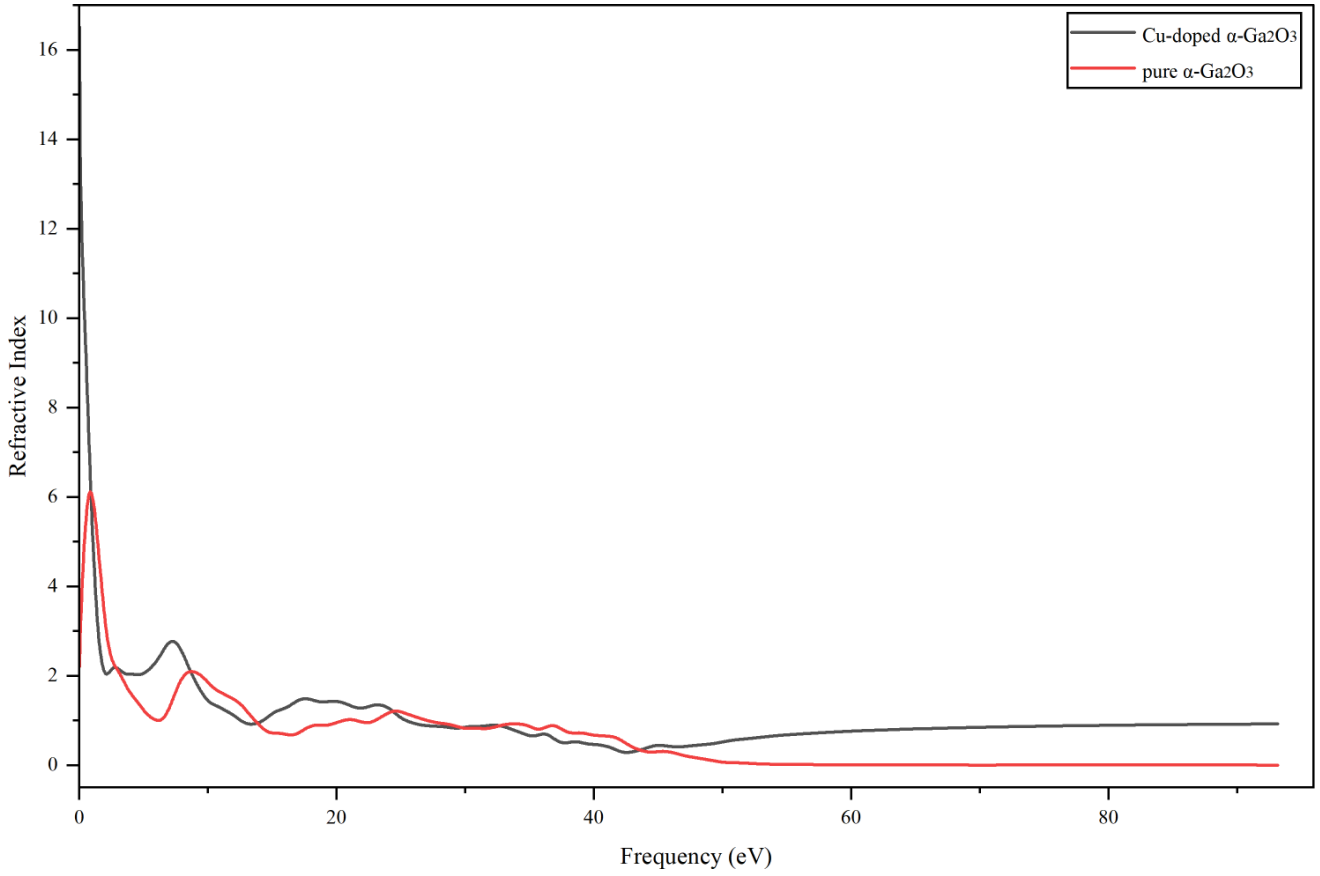


Fig.9: Refractive index of pure and Cu-doped α-Ga_2O_3

5) Loss Function: The energy spent by an electron while ploughing through a medium is called the Loss function. Figure 12 shows the energy loss function (ELF) of pure and Cu-doped α-Ga_2O_3 with respect to frequency (eV). The loss function is characterized by a sharp peak in both samples. The energy loss in Cu-doped α-Ga_2O_3. The pure α-Ga_2O_3 peak in the same region is well over 20 and the highest peak of Cu-doped α-Ga_2O_3 is below 20 in the UV region. This, in turn, means improved optical and electronic devices, for example, UV sensors and filters.

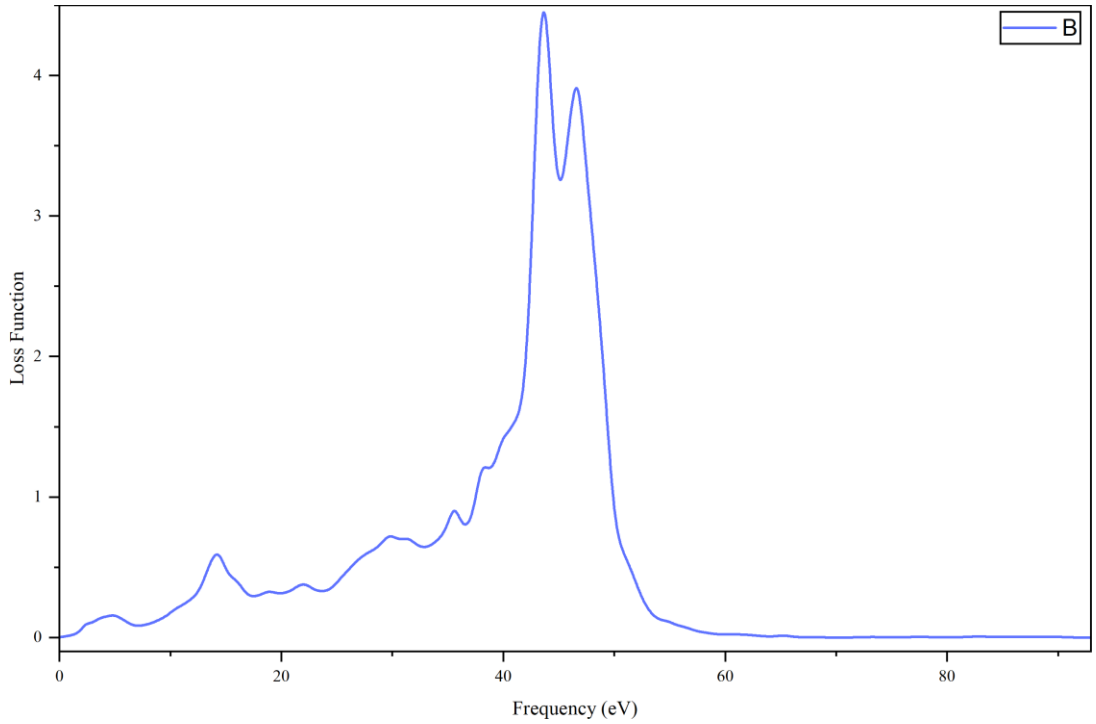


Fig.10: Loss Function of Cu-doped α-Ga_2O_3

4.2 Discussions

The electronic band structure of Cu-doped α-Ga_2O_3 undergoes significant changes with respect to undoped α-Ga_2O_3. The electronic states around the Fermi energy are redistributed due to the changes in the valence and conductive bands that result from the inclusion of Cu atoms. These modifications manifest as a shift in the conduction band edge status indicating possibility of reduced bandgap structure. In doped systems, in particular, the Cu 3d states contribute a significant weight to the electronic density of states (DOS) at (near-)Ef . The observed Fermi level shift in Cu-doped α-Ga_2O_3 is a key result. At low doping Cu mainly hybridizes with the oxygen 2p orbitals, and the change of electronic states occurs. However, the Cu 3d states localize more strongly when the doping increases, and hence contribute to the electronic structure more directly at higher doping concentration. Downshift of the mobility is attributed to the localization of the carriers in the Cu-doped α-Ga_2O_3. This is attributed to the spatial extent of the Cu 3d states which might lead to electron scattering at higher Cu contents. Moreover, by employing the Cu doping, the defect states in the band gap are introduced, and these states may act as trap centers. These states which can act as recombination centers, may affect the electronic characteristic of the material such as conductivity and carrier mobility.

The optical constants of Cu-doped α-Ga_2O_3 have been studied based on the calculated dielectric function and obvious variations are observed with the achieved copper doping. The existence of Cu as the lattice component has a dramatic effect on the

absorption spectrum of α-Ga_2O_3. The absorption edge is red shifted that shows decrease in the optical bandgap of the material due to Cu-doping as clearly seen. This is consistent with the experimental decrease of electronic gap from band calculations. In particular, Cu-doped α-Ga_2O_3 exhibits increased visible light absorption relative to nondoped α-Ga_2O_3. This improvement is considered to result from the supplementary Cu-related electronic states and the novel absorption channels on the visible light. This high visible light absorbance suggests that Cu-doped α-$Ga_2O_3$is a superior candidate for opto electric devices and also in devises that function on the visible range of light. In addition, refractive index and extinction coefficient of Cu-doped α-Ga_2O_3 exhibit clear deviations from the pure α-Ga_2O_3. These modifications indicate that the Cu- doping does not only impact on the electronic transitions but also changes the light- matter interaction in the material. The change to these optical constants may be useful for the construction of materials for optical coatings, sensors, and other optoelectronic devices.

CHAPTER 5
PROJECT MANAGEMENT

5.1 Task, Schedule & Milestones

1. Poject Planning and Initial Research (Week 1-2)

Task 1.1: Define project objectives and scope.

Task 1.2: Conduct literature review on hybrid renewable energy systems.

Task 1.3: Identify and engage stakeholders.

Milestone 1: Completion of project plan and stakeholder engagement.

2. Site Assessment and Resource Evaluation (Week 3-4)

Task 2.1: Site analysis for wind and solar resource assessment.

Task 2.2: Gather data (wind patterns and solar irradiance) and develop the models.

Task 2.3: Evaluate site -specific limitation sand opportunities.

Milestone 2: Finish with Site Survey and Resource Assessment Report.

3. System Design and Component Selection (Week 5-7)

Task 3.1: Sketch the hybrid system layout (wind turbine PV array).

Task 3.2: Choose Equipments (wind turbines, PV panels, batteries, inverters, and charge controllers.

Task 3.3 Writing Detailed Schematics and Specifications for Each System.

Phase 3: Completion of design, and purchase of components.

4. System Installation and Integration (Week 8-10)

Task 4.1: Implementation of wind turbines and PV panels.

Activity 4.2: Install publication battery storage and inverters.

Task 4.3: Incorporation of controllers and charge controllers.

Stage 4: A system installed and integrated.

5. Testing and Optimization (Week 11-12)

Task 5.1: Preliminary system the performance of and testing.

Task 5.2: Tuning and optimization of system components for gain improvements.

Task 5.3: Delivery of intelligent energy management approaches.

Top 5 Milestone: Testing and optimization phase is done.

6. Monitoring and Evaluation (Week 13-14)

Task 6.1: Observe performance and energy produced by the system.

Task 6.2 Determine the reliability and the efficiency of the system.

Task 6.3 Analyse data and conduct corrective actions.

Milestone 6: End of the line performance evaluation and report on finishing

7. Project Closure and Future Recommendations (Week 16)

Task 7.1: Project review meeting with stakeholders.

Task 7.2: Identify possible points in program transfer to scaling.

Task 7.3: Close Project and ensure all output is deliverable.

Deliverable 7: Report on project closing and recommendations for the future.

5.2 Resources and Cost Management

A number of human and technological resources were essential to successfully carrying out this study. The main resources used in this study are computational codes, laboratory facilities, and human knowledge in theoretical physics, computational chemistry, and materials science. Each of these resources was incredibly helpful in the development of the project. The first-principle calculations of this work were performed using CASTEP software package, and relied heavily on HPC facilities. All computations have been performed on clusters of supercomputers, made available by the university, optimized for massive quantum mechanical simulations. These were machines with many cores. These machines were capable of handling complex material simulations, specifically in the study of doping effects at the atomistic level, and were equipped with high-end processors (i.e., Intel Xeon or AMD EPYC) and large memory capacity (e.g., 128GB RAM or higher). Software CHE Group Library code In order to perform the electronic structure calculations and simulations, the widely used first principle software program CASTEP as implemented by density functional theory (DFT) was used as the main software. The electronic properties, band structures and optical properties of Cu-doped α-Ga_2O_3 were calculated by the software here. Other software components like VESTA for visualization and Matlab or Python for data post- processing were needed, too.

Computation is always demanding when using high-performance computing, specially in the case of using supercomputing clusters as they consume a lot of time. The necessary computational facilities were expensive but free access to these was provided using university resources. This reduced the total project cost considerably. Since we performed this research as part of an academic project, the researcher did not have to get a direct economic compensation. However, project time was estimated based on a per hour labor rate calculated for a Ph. is a Ph.D. candidate at the Department of Media and Communication. Minor expenses such as printing, paper, and the obtaining of out-of-print works not open to free consultation, fell to be incurred. These were not massive or unaffordable sums and did not blow the overall budget.

5.3 Lesson Learned

Time Management: The influence of the time management was the vital thing learned in this task. It turned out that the time required for high-performance computing simulations was initially underestimated, thereby causing delays. Better planning with the release of store deadlines for each phase of the work and computation time was the immediate impact of the project. Simultaneous data analysis and planning simulations allowed constraints to be minimized and the efficiency of the project to be improved.

Resource Management: The success of the project depended on how the resources were managed. While computing was readily at hand at the university, computing-intensive simulations were monitored to ensure their interactions were optimized and kept cost-efficient. For future projects, it would have been beneficial to create detailed resource plans including alternatives in case of unexpected scheduling conflicts or resource unavailability.

Collaboration and Communication: The project reinforced the need for collaboration. Research goals were defined and unforeseen challenges were discussed on a weekly basis with faculty advisors, computational experts and researchers in related fields. It was important to keep a constant feedback going on between parties to sort out the issues and improve the quality of research as a whole.

CHAPTER 6

IMPACT ASSESSMENT OF THE PROJECT

6.1 Economical, Societal and Global Impact:

The macroscopic organization of CSNs enables active routing and dynamical computability, and therefore has technological potential to demonstrate synaptic-like behaviors that are important for learning and memory. The semiconductor industry could benefit from the research results about Cu-doped α-Ga_2O_3 which will help to develop new materials for optoelectronics, photo-detectors and PV. Through understanding of the influence of dopants on electronic structure, manufactures will be able to optimize material synthesis to produce high-performance semiconductors in a cost-efficient way. The proposed research has a high potential for creating economic advancement in the medical diagnostics, renewable energy, and electronic devices industries by opening new markets for the advanced material technologies. The discovery of new effects of Cu-doped α-Ga2O3 can be transformed into development of new applications of social benefit, such as photodetectors of higher sensitivity and solar cells of higher efficiency. Potentially creating new jobs in R&D and manufacturing as the demand for materials science and semiconductor industry professional surges. If Cu-doped α-Ga_2O_3 proves suitable for environmentally friendly energy technologies (e.g., solar panels), it can help spur the world-wide adoption of green energy sources. There are opportunities to enhance global cooperation in materials science research, to link nations together and share scientific advances.

6.2 Environmental and Ethical Issues

When doping with copper the impact of copper extraction on the environment should be considered. To minimize the environmental impact, it might be worth exploring environmentally friendly extraction procedures or recycling of copper from e waste. The possible toxicological implications of the use of dopants in electronic devices have to be carefully considered. For instance, unintended emissions from α-Ga2O3-based devices must be addressed due to the potential harm to public health or environment. Correct recycling procedures need to be put into place to avoid environmental contamination when the doped semiconductor materials are disposed of, especially at the end of their life cycle.To avoid monopolistic behaviour commitment must also be made to ethical concerns related to patents, propriety technologies, and on ensuring

equitable access to the research outputs especially for low-income countries that might benefit from the technology. With respect to worldwide access to renewable energy devices or medical technology, the influence of developing technologies should be just, so that no group is privileged over another.

6.3 Utilization of Existing Standards or Codes

It is a matter of standard practice for computations in material science, as stated in ISO 80000 or equivalent international standards, to use the computational tool (ab-initio CASTEP), and that a "property" of the (theoretical) material object is the object of most general standard (microscopic or macroscopic) interest. The initiative follows academic and ethical codes prevailing at the time, among others, the responsible conduct of research (e.g., Nuremberg Code and Helsinki Declaration in biomedical research, where appropriate). This work may provide input to standardization activities dedicated to doped semiconductors, as well as to the commercial application, testing and production processes of the materials. The research could modify or improve the existing standards for semiconductors and optoelectronic devices, which have been defined by bodies such as the ASTM or the IEC.

6.4 Other Concerns

Despite the promising results of the present study, the translation gap between the observed findings of the simulations and industrial level scale applications remains open. The scaling up from laboratory preparation to large scale production requires extra betterment in both process optimization and fabrication process, as well as technical problems to be solved. Regulatory approvals (as, e.g., FDA, CE marking) might be needed for commercialization if the results are used in the development of new consumer or medical devices. Such material should be carefully considered when being brought to the attention of the regulatory authorities for the products in question. The application of new technologies typically depends much on public acceptance, particularly if they pose health, safety, or environmental risks. Through involving the stakeholders, and educating the public from an early stage, any resistance to the new materials and technologies could be overcome.

CHAPTER 7

CONCLUSIONS AND RECOMMENDATIONS

7.1 Conclusions

The optical, and electronic properties of pure and Cu doped crystalline α-Ga_2O_3 have been noticed in this study. By means of the first principal method, the lattice parameter, cell volume, and angle of both pure and Cu-doped α-Ga_2O_3 were figured out at GGA-PBE from the loss function of the material. According to our electronic structure investigation, the main reason for the sharp decrease of the bandgap values from 2.876 eV (pure) to 1.7496 eV (Cu-doping) is the presence of Cu 3d states, which can lead to impurity levels which hybridize with O 2p and Ga 4p orbitals and are located just below the valence band. This also results in enhanced carrier excitation and tunability in an electronic application. Substantial change in optical properties such as reflectance, absorption and dielectric function is presented by Cu doping. Considering with the shift of an absorption edge towards a red and the increased absorption in the UV region, it is suggested that Cu-doped α-Ga_2O_3 may be one of the good candidates for UV photodetectors and T-oxidation electronics. After Cu doped, the reflectivity reveals stronger light-matter coupling, and possible more convenient applications in optoelectronic are expected due to the doped dielectric function. The possible use of UV sensors is suggested by the Cu-doped increased conductivity and low loss function. However, the simulation and analysis can be subject to limitations or be flawed, with the results becoming invalid. Therefore, more comprehensive studies need to be conducted to improve the results and to allow comparisons with other relevant research in this domain.

7.2 New Skills and Experiences Learned

The following skills and values occurred during this course of study and assisted the development of the student as well as the student:

An important insight was also provided by adopting the CASPEST first-principles calculation to computational material science. This comprises knowledge of density functional theory (DFT), investigation in electronic structures, and the description of the optical properties from first-principle calculations. Studies into doped semiconductors, particularly Cu-doping in α-Ga_2O_3, have clarified how doping changes electrical and optical properties of a material. This knowledge is necessary to fabricate materials with desired properties for specific applications. The analysis of computational data, i.e., optical spectra, band structure, density of states (DOS) and dielectric functions, provided valuable experience in the inference of relevant details from complex data. A key goal was for students to have a mindset to ask questions and compare data to prior collected experimental data. Writing this thesis further developed my understanding of adhering to academic protocols, structuring a research paper, and clearly presenting results. Value for future studies and publishing efforts is invaluable. To use the research process, I had to solve problems related to computing limitations,

model accuracy, and understanding complex results. It developed problem solving skills and critical thinking, particularly in the area of computational materials science.

7.3 Future Recommendations

The following recommendations for future work are issued in the context of what the research concludes and the challenges it has faced:

Even if the computational results provide valuable information, it is important to verify such conclusions with experimental techniques, such as Photoluminescence (PL) measurements, UV-Vis spectroscopy, and X-Ray diffraction (XRD). Experimental verification would enhance the practical applicability of the findings. The doping effects (with other elements other than La and Al, e.g., Ni, Zn, and Co) on the electrical and optical properties of α-Ga_2O_3might also be interesting to investigate to broaden the understanding of how different doping elements influence the electronic and optical properties of this material. Additional adjustment of the material characteristics could potentially be achieved by examining the effect of co-doping the system with other transition metals. Further works can be performed to systematically tune the Cu-doping concentration and to explore its impact on the functionality of the material (especially in optoelectronic devices). This will identify the optimum doping concentration for maximizing the characteristics of interest. A more detailed examination of the effects of point defects and impurity states on the electrical and optical properties of Cu-doped α-Ga_2O_3 may be required. Moreover, understanding defects could help in the development of more efficient devices, as they can strongly influence a material's performance in optical and electrical applications.

The possibility of fabricating hybrid systems or heterostructures based on Cu-doped α-Ga_2O_3, created by coupling it with other materials (such as graphene or other 2D systems) is convincing to expand the overall performance of the material, in challenging optoelectronic and photovoltaic applications. Future work shall focus on the fabrication and testing of Cu-doped α-Ga_2O_3 saeson-basedd devices. The direct observation was helpful to evaluate its practical application, such as whether it is possible to be large-scale, stable, and efficient for real business.

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