

**“Modifications in inorganic oxides for the application in
electronic devices with semiconductors”**

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I/We Tanya Mehra and Riya Chaudhary hereby certify that the work which is being presented in the dissertation entitled “**Modifications in inorganic oxides for the application in electronic devices with semiconductors**” in partial fulfilment of the requirements for the award of the Degree of Master of Science in Chemistry, submitted in the Department of Applied Chemistry, Delhi Technological University is an authentic record of our own work carried out during the period from 2022 to 2024 under the supervision of Prof. Roli Purwar.

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Certified that Tanya Mehra and Riya Chaudhary have carried out their research work presented in this dissertation entitled “**Modifications in inorganic oxides for the application in electronic devices with semiconductors**” for the award of **Master of Science in Chemistry** from Department of Applied Chemistry, Delhi Technological University, Delhi, under our supervision. The dissertation embodies results of original work, and studies are carried out by the students themselves and the contents of the dissertation do not form the basis for the award of any other degree to the candidates or anybody else from this or any other University/Institution.

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Abstract:

This dissertation examines the alterations made to inorganic oxides in order to improve their usability in electronic devices that include semiconductors. Inorganic oxides, renowned for their distinctive electrical, optical, and thermal characteristics, play a vital role in the advancement of semiconductor technology. Nevertheless, the performance of these systems may be constrained by intrinsic material characteristics. This study investigates many methods, like as doping, nanostructuring, and surface treatments, to enhance the performance of these oxides for electronic purposes. The thesis conducts a thorough analysis of current literature and experimental experiments to identify crucial techniques for enhancing the conductivity, stability, and integration compatibility of inorganic oxides.

More precisely, ZnO nanoparticles that were pure and doped with Fe were synthesized using a cost-effective co-precipitation technique. The optical characteristics of the materials were investigated using UV-Vis absorption spectroscopy. The results showed that pure ZnO had a band gap of 3.420 eV. For ZnO with 2%, 5%, and 10% Fe doping, the band gaps were measured to be 3.23 eV, 3.57 eV, and 3.07 eV, respectively. An increase in doping concentration resulted in a shift of the measured wavelength from 373 nm to 368 nm, known as a blue shift. The work demonstrates that the optical and electrical characteristics of Fe-ZnO nanoparticles are contingent upon the sizes of the particles, as determined by analyzing zeta potential and particle size data.

Keywords: Semiconductors, Inorganic Oxides, UV-Vis Absorption, ZnO Nanoparticles

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List of abbreviations

RD - X-ray diffraction

SEM - Scanning electron microscopy

SiO₂ - Silicon dioxide

TiO₂ - Titanium dioxide

ZnO - zinc oxide

ITO - Indium tin oxide

TCO - Transparent conductive oxide

FETs - Field-effect transistors

TFTs - Thin-film transistors

IGZO - Indium gallium zinc oxide

FT -IR - Fourier Transform Infrared

XPS - X-Ray Photoelectron Spectroscopy

TEM - Transmission Electron Microscopy

NaOH - Sodium hydroxide

FeCl₃ - Ferric chloride

Chapter – I Introduction

In the rapidly evolving field of electronics, there is a growing need for devices that provide exceptional performance, reliability, and efficiency. Semiconductors are the essential building blocks of contemporary electronic devices, providing the basis for the operation of many electronic gadgets, including high-performance computers and smartphones [1, 2]. The unique attributes of inorganic oxides, including their exceptional thermal stability, broad bandgaps, and remarkable dielectric properties, have resulted in their vital role as indispensable materials in the domain of semiconductor technology [2]. It is typical for inorganic oxides to necessitate modifications in order to enhance their compatibility and performance in electronic applications. This is essential to properly maximize the advantages they provide [2, 3 & 4].

Photocatalytic technique is one way that utilizes semiconductors to degrade organic dyes [1]. Using zinc oxide-based photocatalysts to remove organic pollutants from water by UV light irradiation is an encouraging strategy. Zinc oxide is an attractive semiconductor photocatalyst due to its wide bandgap of 3.366 eV.

Additionally, ZnO-based semiconductors have limited use due to their elevated charge carrier recombination rate. To stop the recombination of photogenerated electron and hole pairs, nanosized materials based on ZnO have commonly used transition metals as dopants due to their abundance and relative cheapness. The iron's three-dimensional orbitals are quite interactive, making it an attractive option for the ZnO lattice. The method used here is based on the co-precipitation strategy, however there are other approaches to generate Fe-doped ZnO nanoparticles as well.

The combination of inorganic oxides with semiconductor devices can be impeded by their inherent properties, hence reducing their effectiveness. Modifying these materials necessitates innovative approaches due to challenges such as poor conductivity, unstable interfaces, and insufficient electrical properties [3, 4]. This thesis explores various modification ways to overcome these challenges and enhance the performance of inorganic oxides for use in electrical devices [4]. Research is now investigating approaches such as doping, nanostructuring, and surface treatments to enhance key metrics including thermal stability, electrical conductivity, and interface quality [5].

The primary aim of this study is to offer a comprehensive evaluation of the present condition of inorganic oxides in semiconductor applications, with the objective of emphasizing the main limitations and challenges currently being encountered [5, 6]. Secondly, it examines various modification processes and evaluates the effectiveness of these strategies through several experimental trials [7]. Lastly, its aim is to offer a set of guidelines and optimal methods for tailoring inorganic oxides to meet the specific needs of various electronic applications [8].

The significance of this dissertation lies in its potential to drive advancements in electrical device technology. Enhancing the characteristics of inorganic oxides can lead to the creation of more efficient and reliable semiconductors [6]. Ultimately, this will lead to enhancements in the efficiency of equipment and their durability. This thesis will not only contribute to the existing knowledge in materials science and electrical engineering, but it will also provide valuable insights that can potentially lead to the development of advanced electronic devices with superior performance [5, 6 & 7].

1.1. Background:

Inorganic oxides have become indispensable in semiconductor technology due to their unique and versatile characteristics. Various electrical devices utilize a wide range of materials, including SiO₂, TiO₂, and ZnO. These materials are employed in transistors, sensors, and capacitors [2, 4]. These materials are suitable for applications that require long-lasting and dependable performance under many conditions due to their wide bandgaps, high dielectric constants, and thermal stability [5].

Nevertheless, despite the advantageous characteristics of inorganic oxides, the integration of these substances into semiconductor devices has some challenges [4, 6]. The primary issues that require attention are the restricted electrical conductivity, potential contact defects, and instability in certain operating situations. In order to mitigate the potential adverse effects of these limitations on the efficiency and longevity of electronic devices, it is imperative to develop techniques that can alter and enhance the characteristics of these oxides [7].

Several modification techniques, such as doping, nanostructuring, and surface treatments, have shown promise in addressing these challenges [6]. Doping involves introducing impurities to alter electrical and optical properties, nanostructuring aims to enhance surface area and reactivity, and surface treatments aim to improve interface stability [7, 8]. For

instance, the addition of aluminum to zinc oxide can significantly enhance its conductivity, whereas the process of nanostructuring titanium dioxide can increase its efficiency in catalysing reactions with light, which is beneficial for the development of sensors. Both of these methodologies contribute to the advancement of novel materials [8, 9 & 10].

Implementing these tweaks could lead to substantial enhancements in device performance. Enhanced inorganic oxides possess the capacity to generate charge carriers that are highly efficient, provide more effective thermal control, and provide more reliable device operation [8]. Given the increasing complexity and miniaturization of electronic equipment, it is imperative to make these advancements. The reason for this is that the gadgets necessitate materials that can function consistently at smaller dimensions and under more challenging circumstances [9, 10].

The main goals of this thesis are to thoroughly examine various modification procedures, assess their effectiveness through experimental study, and understand the impact these techniques have on the functionality of electronic equipment [9]. The objective of this research is to enhance the properties of inorganic oxides for semiconductor applications by investigating how alterations in these materials can contribute to the development of electronic materials and the creation of next-generation electronic devices [10, 11].

1.2. Research Aim & Objectives:

1.2.1. Research Aim:

The research aims to enhance the performance of inorganic oxides in semiconductor applications by exploring modification techniques such as doping, nanostructuring, and surface treatments [8, 11]. This involves evaluating their impact on electrical, structural, and optical properties to improve device efficiency, stability, and integration compatibility.

1.2.2. Research Objectives:

1. To evaluate the current limitations and challenges of inorganic oxides in semiconductor applications through a comprehensive literature review.
2. To investigate the effectiveness of modification techniques, including doping, nanostructuring, and surface treatments, on improving the properties of inorganic oxides.

3. To conduct experimental studies using advanced characterization techniques to assess the impact of these modifications on the performance of electronic devices.

1.3. Research Questions:

1. What are the main limitations and challenges faced by inorganic oxides in semiconductor applications?
2. How do modification techniques such as doping, nanostructuring, and surface treatments affect the electrical, structural, and optical properties of inorganic oxides?
3. What are the specific impacts of these modifications on the performance and integration compatibility of electronic devices incorporating inorganic oxides?

1.4. Problem statements:

In the rapidly evolving field of electronics, the integration of inorganic oxides with semiconductor devices is essential for achieving high performance, reliability, and efficiency [5]. Inorganic oxides, such as SiO₂, TiO₂, and ZnO, are valued for their exceptional thermal stability, broad bandgaps, and remarkable dielectric properties [9, 10]. However, these materials face significant challenges that limit their effectiveness in electronic applications [10]. The inherent low electrical conductivity, potential contact defects, and instability under certain operating conditions impede their seamless integration with semiconductor devices, reducing overall device performance and longevity [11, 12].

Addressing these challenges requires innovative modification techniques. Doping, nanostructuring, and surface treatments have shown promise in enhancing the properties of inorganic oxides, yet comprehensive studies are needed to understand their full potential and limitations [12, 13 & 14]. Furthermore, there is a lack of systematic guidelines for optimizing these modifications to meet the specific requirements of various electronic applications.

This thesis aims to bridge this gap by exploring and evaluating different modification strategies to improve the electrical, structural, and optical properties of inorganic oxides [13]. By employing advanced characterization techniques, this research seeks to provide a thorough understanding of how these modifications can enhance device performance, ultimately contributing to the development of more efficient and reliable next-generation electronic devices [14, 15].

1.5. Rational:

The rationale for this research lies in the critical need to advance the performance and reliability of electronic devices by optimizing the properties of inorganic oxides used in semiconductor applications [10]. Inorganic oxides such as SiO₂, TiO₂, and ZnO are fundamental materials in the electronics industry due to their unique thermal stability, broad bandgaps, and excellent dielectric properties [11]. However, their inherent limitations, including low electrical conductivity and interface instability, hinder their full potential in enhancing device performance [14].

As electronic devices continue to shrink in size and increase in complexity, the demand for materials that can perform reliably under stringent conditions grows [14]. Traditional approaches to material improvement have reached their limits, necessitating innovative modification techniques [15]. Doping, nanostructuring, and surface treatments offer promising avenues to address these challenges by enhancing the electrical, structural, and optical properties of inorganic oxides [15].

This research is crucial as it aims to systematically investigate and evaluate these modification techniques, providing a deeper understanding of their effects on material properties and device performance [15, 16]. The insights gained will contribute to the development of next-generation electronic devices with superior efficiency, stability, and functionality, ultimately driving innovation in the semiconductor industry and meeting the ever-evolving demands of modern technology [15, 16 & 17].

1.6. Significance of Study:

The significance of this study lies in its potential to revolutionize the application of inorganic oxides in semiconductor technology, thereby advancing the performance and reliability of electronic devices [16]. Inorganic oxides, such as SiO₂, TiO₂, and ZnO, play a crucial role in the functionality of semiconductors due to their unique properties [17]. However, their inherent limitations, including low electrical conductivity and interface instability, restrict their effectiveness in high-performance applications [18].

This research addresses these challenges by exploring modification techniques such as doping, nanostructuring, and surface treatments to enhance the properties of inorganic oxides [18]. By employing advanced characterization methods like XRD, SEM, and electrical testing,

the study provides a comprehensive evaluation of how these modifications impact the electrical, structural, and optical properties of inorganic oxides [18, 19].

The findings from this research are expected to lead to significant improvements in the efficiency, stability, and integration compatibility of electronic devices [18]. This will not only enhance the performance of current technologies but also pave the way for the development of next-generation devices, including transistors, sensors, and memory devices [19]. Ultimately, the study's contributions will drive innovation in the semiconductor industry, providing valuable insights and practical guidelines for future research and development efforts in electronic materials science [20, 21].

1.7. Research limitations:

While this research aims to explore and optimize modifications in inorganic oxides for semiconductor applications, it is important to acknowledge several limitations that may affect the scope and applicability of the findings [18]. Firstly, the study focuses on a select group of inorganic oxides, primarily SiO₂, TiO₂, and ZnO. This limitation means that the results may not be directly applicable to other inorganic oxides with different properties and behaviours [18, 19, 20 & 22].

Secondly, the modification techniques investigated doping, nanostructuring, and surface treatments are complex processes that require precise control and may vary in effectiveness depending on the specific conditions and materials used [20, 21]. The scalability of these techniques from laboratory settings to industrial applications poses a significant challenge, as reproducibility and consistency are critical for commercial viability [22].

Additionally, the advanced characterization techniques employed, such as XRD, SEM, and electrical testing, provide detailed insights but may not fully capture all aspects of material behavior under operational conditions [23]. Real-world applications often involve varying environmental factors, such as temperature fluctuations and mechanical stress, which may not be thoroughly simulated in experimental settings [24].

Finally, the interdisciplinary nature of this research necessitates a comprehensive understanding of materials science, electrical engineering, and nanotechnology [22, 23 & 24]. This complexity may limit the ability to address all potential interactions and outcomes comprehensively. Future studies should aim to expand the range of materials and techniques

explored, improve scalability, and incorporate more extensive real-world testing to validate and build upon the findings of this research [25].

1.8. Thesis Organization:

This is the thesis's outline: The introduction will be covered in Chapter 1. A thorough review of the literature is provided in Chapter 2, which also highlights research gaps that this study aims to fill and summarises previous findings. Chapter 3 provides specifics on the procedures, including the instruments and strategies used for modifications. Chapter 4 examines the effects of various modifications on the properties of inorganic oxides and includes a discussion of the results. A summary of the key findings, a discussion of their importance, and suggestions for additional research are included in the fifth and final chapter.

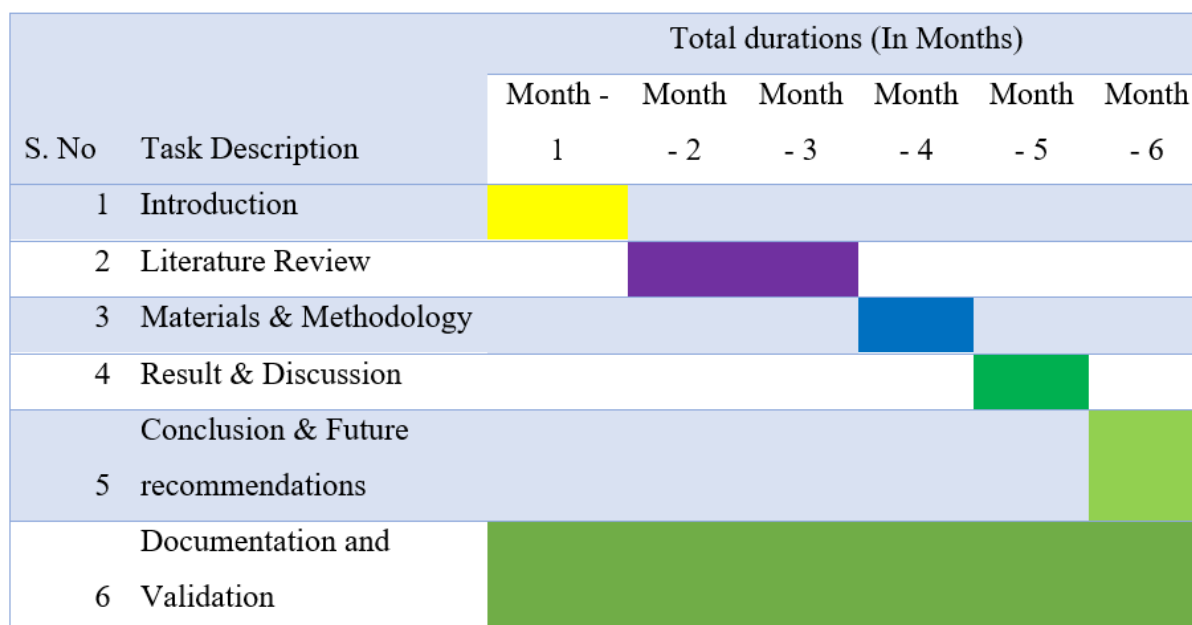


Figure.1.1. Gantt chart of the research plan

Chapter – II Literature Review

The literature review offers a comprehensive overview of the current level of knowledge in the field of inorganic oxides utilised in semiconductor applications by analysing historical trends, key discoveries, and recent developments [2, 3]. Many electrical devices rely on inorganic oxides because of their exceptional dielectric properties, thermal stability, and large bandgaps [2, 3 & 4].

The review begins by examining the historical development of inorganic oxides in semiconductor technology, tracing their evolution from early discoveries to their present-day applications [4]. Key milestones and breakthroughs are highlighted to provide context for understanding the current research landscape [5]. Recent advances in semiconductor technologies are then explored, with a focus on the integration of inorganic oxides with semiconductor devices [6, 7]. This includes discussions on the challenges and opportunities associated with incorporating inorganic oxides into electronic components such as transistors, sensors, and capacitors [8, 9 & 10].

The review also delves into the theoretical background of semiconductor physics and electronic properties of inorganic oxides, providing readers with a foundational understanding of the underlying principles governing their behavior [11]. Key concepts such as band theory, carrier transport, and interface phenomena are discussed in detail to elucidate the mechanisms driving the performance of inorganic oxide-based semiconductor devices [10, 11, 12 & 13].

Furthermore, the review examines various modification techniques employed to enhance the properties of inorganic oxides for semiconductor applications [14]. These techniques include doping, nanostructuring, and surface treatments, each offering unique advantages for improving conductivity, stability, and integration compatibility [15, 16, 18, & 25]. Overall, the literature review synthesizes existing knowledge and identifies gaps in understanding, laying the groundwork for the subsequent research objectives and methodologies outlined in the thesis [16, 19, 22 & 27].

2.1. Theoretical framework:

2.1.1. Overview of Inorganic Oxides:

Inorganic oxides constitute a diverse class of materials with wide-ranging applications in electronics. SiO₂, TiO₂, and ZnO are prominent examples known for their unique properties

[12]. These oxides possess attributes like high thermal stability, wide bandgaps, and exceptional dielectric properties, making them indispensable in semiconductor technology [13, 14 & 18]. Their crystalline structures and chemical compositions vary, allowing for tailored properties to suit specific applications. Inorganic oxides serve as insulators, capacitors, and protective coatings, contributing to the functionality and reliability of electronic devices [19, 20 & 21]. Understanding their structural, electrical, and optical characteristics is essential for optimizing their performance in semiconductor applications [23].

2.1.2. Properties and Applications of Inorganic Oxides in Electronics:

Inorganic oxides offer a myriad of properties that are crucial for electronic applications. Their high thermal stability ensures device reliability under extreme operating conditions. Wide bandgaps make them suitable for semiconductor materials, enabling efficient electron transport and minimizing leakage currents [11]. Exceptional dielectric properties facilitate the storage and transmission of electrical energy in capacitors and insulating layers [17, 18]. These properties find applications in various electronic components such as transistors, sensors, and memory devices [19]. For instance, SiO₂ is extensively used as a gate dielectric in MOSFETs, while ZnO is employed in transparent conductive coatings for displays and solar cells [24]. Understanding the relationship between oxide properties and device performance is crucial for advancing electronic technologies [25].

2.1.3. Historical Development and Key Discoveries:

The historical development of inorganic oxides in electronics traces back to early discoveries of their properties and applications [11]. SiO₂ emerged as a key material in semiconductor technology due to its excellent insulating properties and compatibility with silicon substrates [15, 17]. TiO₂ gained attention for its photocatalytic properties and potential applications in photovoltaics and sensors [19]. ZnO garnered interest for its wide bandgap and piezoelectric properties, leading to advancements in optoelectronics and sensors. Over time, researchers made significant discoveries regarding the synthesis, characterization, and manipulation of oxide materials, paving the way for innovations in electronic devices [25].

2.1.4. Recent Advances in Semiconductor Technologies:

New inorganic oxide materials and architectural advances in semiconductor devices have driven the industry forward at a dizzying pace in the last several years [19]. Constant efforts to

shrink the size of electronic components, such as transistors, have spurred the development of new materials and manufacturing processes [22]. By enabling exact control over oxide structures and properties, nanotechnology has opened up new paths for device integration and performance enhancement [24, 25 & 29]. The development of novel applications, like flexible and wearable electronics, has prompted research into oxide-based materials that can have their mechanical and electrical properties modified [22]. Research into semiconductors faces new opportunities and challenges as a result of their integration with emerging technologies including quantum computing, the IoT, and artificial intelligence (AI) [23].

2.1.5. Integration of Inorganic Oxides with Semiconductors:

Integrating inorganic oxides with semiconductors improves the functionality and performance of electronic devices. In semiconductor devices, oxides serve as gate dielectrics, passivation layers, and active components [16]. Compatibility with semiconductor substrates and manufacturing techniques is crucial for trustworthy device performance. Integration issues, including as interface engineering, defect reduction, and process compatibility, must be addressed before oxide-semiconductor systems may be used to their full potential [18, 19 & 27]. Research into optimising oxide properties primarily aims to improve device functioning, energy efficiency, and reliability [21]. Methods like device design, surface modification, and material engineering are being used to achieve this optimisation. The advancements in oxide-semiconductor integration have opened the door to next-generation electronic devices that will revolutionise sensing, communication, computing, and other areas [25, 26].

2.1.6. Semiconductor Physics:

The study of materials with semiconducting properties and how they behave is known as semiconductor physics. The inorganic oxides SiO_2 , TiO_2 , and ZnO are all part of these materials. At its heart, semiconductor physics is about understanding how semiconductor devices work, band theory, and carrier transport [24]. The bandgap, which is what defines a material's conductivity, and the formation of valence and conduction bands are both explained by band theory [27]. The electrical properties of a semiconductor are determined by carrier transport, which is the movement of charge carriers (holes and electrons) inside the material [28]. To control the flow of electricity, semiconductor devices like diodes and transistors work by changing the positions of carriers [29, 30].

2.1.7. Semiconductor Applications:

The use of inorganic oxides in semiconductor applications has been essential in advancing modern electronic devices, harnessing their unique properties for different purposes [13]. ITO is a type of TCO that is widely acknowledged as an essential element in electronic displays, solar cells, and touchscreens [15]. ITO's distinctive blend of high electrical conductivity and optical transparency allows for efficient light transmission while facilitating electronic conduction [17].

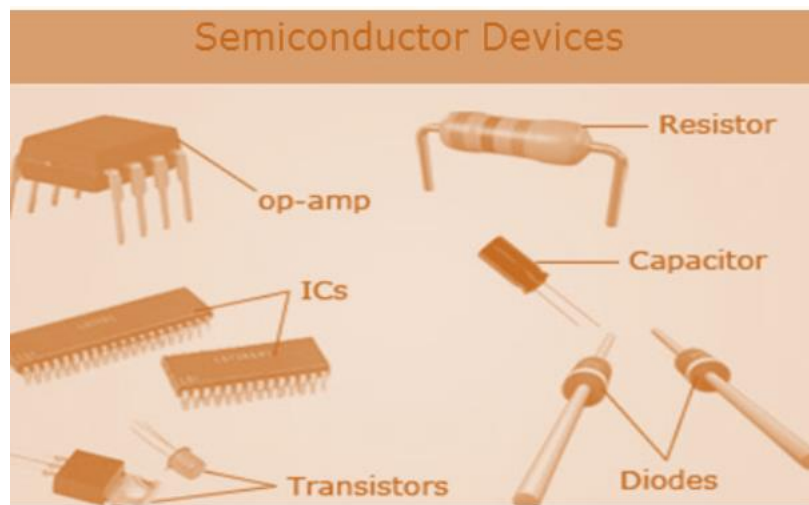


Figure.2.1. Model of semiconductor applications

ZnO is a highly efficient semiconductor, particularly when arranged in nanowires, exhibiting excellent electron mobility and a significant surface area [18]. ZnO is very ideal for utilisation in FETs and sensors because of its versatile nature and ability to be adjusted [24]. The popularity of TFTs has grown due to the introduction of oxide semiconductors like IGZO. These materials have exceptional electron mobility and stability, making them essential for display technologies and flexible electronics [25]. IGZO and TFTs provide exceptional performance and energy efficiency in various applications, including flat-panel displays [26].

The incorporation of inorganic oxides in semiconductor applications is a pivotal intersection of materials science and electronics, propelling breakthroughs in technology [27]. Integrating them into various electrical components not only enhances device performance but also adds to the development of energy-efficient and cutting-edge technologies that define our contemporary digital world [28].

Table.2.1. List of applications of semiconductors

S. No.	Semiconductor	Applications
1.	Transparent Conductive Oxides (TCOs)	A well-studied TCO is commonly used as a transparent electrode in many electronic goods, such as solar cells and flat-panel displays. Because of its high optical transparency and exceptional electrical conductivity, it is a crucial part of contemporary electronic systems.
2.	Zinc Oxide (ZnO) Nanowires	ZnO, especially in the nanowire structure, has demonstrated potential in the field of semiconductor applications. ZnO nanowires possess a notable combination of elevated electron mobility and a substantial surface area, rendering them well-suited for use in FETs and sensors. ZnO versatility in synthesis methods enables the customization of its characteristics to fulfil precise device specifications.
3.	Thin-Film Transistors (TFTs)	IGZO is a type of oxide semiconductor that has gained significant interest due to its potential use in thin-film transistors. IGZO TFTs possess superior electron mobility, stability, and transparency, rendering them well-suited for use in displays and flexible electronics.

2.1.8. Electronic Properties of Inorganic Oxides:

The electrical characteristics of inorganic oxides play a vital role in their use in semiconductor technology [21]. The attributes encompass electrical conductivity, dielectric constant, bandgap energy, and carrier mobility [25]. SiO₂ is a very effective insulator with a significant dielectric constant, which makes it well-suited for serving as a gate dielectric in MOSFETs. TiO₂ and ZnO have distinct optical and electrical characteristics, including wide bandgaps and high carrier mobilities. These qualities make them suitable for use in photovoltaics, sensors, and transparent conductive coatings [26, 28].

Inorganic oxides are a diverse collection of compounds that possess a wide range of characteristics, making them crucial in various scientific and technical applications [29]. One notable characteristic is their remarkable structural flexibility, which encompasses a wide range of crystalline arrangements, including polymorphs and nanostructures. Diversity allows for the customisation of characteristics to meet specific application requirements [29, 30].

The electrical properties of inorganic oxides play a critical role in determining their use. Oxides possess intrinsic or modifiable semiconducting characteristics, which are essential for their integration into electrical devices [24, 25]. ITO and ZnO are significant transparent conductive materials because they possess a high level of electrical conductivity and exceptional electron mobility. These materials are essential in a range of applications, such as solar cells, flat-panel displays, and touchscreens [27]. Additionally, the optical transparency of some inorganic oxides is of great importance in the field of optoelectronics [28]. SnO₂ and TiO₂ exhibit transparency in both the visible and ultraviolet spectra, rendering them very suitable for applications in UV filters, optical coatings, and photovoltaic systems [29].

Metal oxides act as catalysts in catalysis due to their redox properties [28, 29]. Transition metal oxides, such as manganese dioxide (MnO₂), are essential catalysts for chemical reactions, highlighting the wide range of functions that inorganic oxides serve in several scientific disciplines. Inorganic oxides exhibit a diverse array of characteristics that render them extremely versatile and indispensable materials for the progress of technology and scientific understanding [30, 31].

2.1.9. Interaction between Oxides and Semiconductors:

The interaction between inorganic oxides and semiconductors is crucial for the performance and reliability of semiconductor devices [21]. Oxides are commonly integrated into semiconductor structures as gate dielectrics, passivation layers, or active components [22, 23]. The interface between the oxide and semiconductor plays a critical role in determining device characteristics such as carrier mobility, threshold voltage, and leakage current [25]. Engineering the oxide-semiconductor interface involves controlling factors such as interfacial charge density, interface roughness, and defect states to optimize device performance. Understanding the mechanisms governing the interaction between oxides and semiconductors is essential for the design and fabrication of high-performance electronic devices [28].

2.1.10. Modification Techniques (Doping, Surface Treatments, Structural Adjustments):

Modification techniques are employed to tailor the properties of inorganic oxides for specific semiconductor applications [19]. Doping involves introducing impurities into the oxide lattice to alter its electrical conductivity or optical properties. Surface treatments modify the surface chemistry and morphology of oxides to enhance their compatibility with semiconductor substrates and improve device performance [23, 28]. Structural adjustments, such as nanostructuring or thin-film deposition, allow for precise control over oxide properties and interfaces [27]. These modification techniques enable the optimization of oxide materials for various electronic devices, including transistors, sensors, and memory devices [29]. By fine-tuning the electronic and structural properties of inorganic oxides, researchers can overcome limitations and enhance the performance of semiconductor technologies [30].

2.2. Conceptual framework:

The conceptual framework of this research revolves around understanding and optimizing the properties of inorganic oxides for their application in semiconductor devices [29]. This framework is built upon several key pillars:

Fundamental Understanding of Inorganic Oxides: Central to the conceptual framework is a thorough comprehension of the properties and behavior of inorganic oxides [22]. This includes their structural, electrical, and optical characteristics, as well as their interactions with semiconductor materials [24]. By elucidating the fundamental principles governing oxide behavior, researchers can identify avenues for enhancement and optimization.

Integration with Semiconductor Physics: Semiconductor physics provides the theoretical foundation for understanding the behavior of semiconductor materials and devices [17, 18]. Concepts such as band theory, carrier transport, and device operation are essential for interpreting the performance of oxide-semiconductor systems. Integrating knowledge of semiconductor physics with the properties of inorganic oxides enables researchers to design and engineer devices with tailored functionalities [32].

Modification Techniques: Modification techniques such as doping, surface treatments, and structural adjustments play a crucial role in tailoring the properties of inorganic oxides to meet the requirements of specific semiconductor applications [32]. These techniques allow

researchers to manipulate the electrical, optical, and structural properties of oxides, enhancing their compatibility with semiconductor substrates and improving device performance [32, 33].

Characterization and Evaluation: Existing characterisation techniques like as electrical testing, XRD, and scanning electron microscopy are used to evaluate the effect of modifications on oxide properties [31, 32]. Research into the structural, electrical, and optical characteristics of modified oxides is necessary before their potential usage in various semiconductor applications can be assessed [34].

Real-world Application and Impact: Ultimately, the conceptual framework aims to translate fundamental research into practical applications with real-world impact [32]. By optimizing the properties of inorganic oxides, researchers can develop semiconductor devices with improved efficiency, reliability, and functionality [33]. These advancements have the potential to drive innovation in electronic devices such as transistors, sensors, and memory devices, contributing to the advancement of semiconductor technology [34].

2.3. Critical Analysis of Existing Literature:

In recent years, there has been a surge in the need for high-performance electronic equipment, particularly semiconductors, as a result of the rapid advancements in technology [13]. The exploration of materials with enhanced electrical properties has been a primary area of study in this specific context [18]. Recently, there has been a growing interest in using inorganic oxides in electronic devices due to their unique electrical, optical, and structural characteristics [21, 24].

Significant progress has been made in utilising inorganic oxides, particularly in semiconductors, for electronic devices [27, 29]. Transparent conductive oxides, oxide nanowires, and thin-film transistors have shown considerable promise in several applications [29]. The current focus of research is centred on addressing stability and reliability challenges, exploring new oxide materials, and applying innovative techniques such as doping and alloying [31, 32]. The development of inorganic oxide materials is crucial for the progress and future of electrical devices.

Table.2.2. A summary of a critical evaluation of the literature

S. No.	Inorganic Oxides	Outcomes	Applications	Ref.
1	Zinc Oxide (ZnO)	Optimization of thin-film transistors, ALD techniques	Transparent Conducting Films, Field-Effect Transistors	6
2	Indium Oxide (In ₂ O ₃)	Exploration of solution processing techniques	Thin-Film Transistors, Transparent Conductive Coatings	8
3	Tin Oxide (SnO ₂)	Gas Sensors, Optoelectronic Devices	Investigation into potential optoelectronic applications	11
4	Perovskite Oxides	Novel materials discovery and integration into electronic devices	Versatile properties for various applications	16
5	Nanowires (NWs)	Presenting critical strategies for photogravure for integration of inorganic functional elements	Electronics, Photovoltaics, Optoelectronics, Catalysis	22
6	Metal Oxide Nanoparticles	Development of metal oxide nanoparticles as semiconductors	Semiconductor Devices, Nanotechnology, Sensors	1
7	Co-Zn-Fe ₂ O ₄ Nanoparticles	Impact of Co ²⁺ substitution on microstructure and magnetic properties	Nanomaterials, Magnetic Devices	16
8	Eu ₂ O ₃ -ZnO Mixed Oxide Nanoparticles	Synthesis, characterization, and photocatalysis enhancement	Photocatalysis, Environmental	17

			Applications, Nanotechnology	
9	Magnetite Nanoparticles	Simple and reliable synthesis of superparamagnetic magnetite nanoparticles	Nanomaterials, Biomedical Applications	24
10	Nano- Biosensors	Relevance of nano-biosensors in tissue engineering	Tissue Engineering, Biomedical Applications, Nanotechnology	23

2.4. Chapter summary:

The literature reviews chapter provides an overview of everything that is currently known about using inorganic oxides in semiconductor applications. Among other significant inorganic oxides, research on silicon dioxide, titanium dioxide, and zinc oxide includes a detailed analysis of their characteristics, uses, and evolutionary history. The latest developments in semiconductor technology and the incorporation of inorganic oxides into semiconductors are also examined.

The paper explores the electrical characteristics of inorganic oxides, semiconductor physics' theoretical foundations, and various modification techniques. This chapter lays out the conceptual framework, reviews the literature critically, and pinpoints knowledge gaps all of which help to shape the direction of upcoming studies. When considered as a whole, the literature evaluation offers a framework for comprehending the importance of inorganic oxide modification and its possible influence on the advancement of electronic device technology.

Chapter – III Materials and Methodology

This chapter provides a detailed description of the preparation, alteration, and characterization of ZnO nanoparticles. ZnO was synthesised using ethanol, deionized water, sodium hydroxide, and zinc acetate dihydrate [22]. After raising the mixture's pH to 8 and heating it to 85 °C, zinc hydroxide was precipitated. The mixture was then dried, cleaned, and annealed at 400 °C. Iron doping was carried out using iron ferrite chloride at Fe concentrations of 2%, 5%, and 10%.

The characterisation approach involved the utilization of UV-Vis-NIR spectrophotometry for band gap measurement, and FTIR spectroscopy for functional groups. To assess the impact of doping on chemical, optical, and structural characteristics, one can compare the properties of pure ZnO with those of ZnO doped with Fe [28].

3.1. Chemicals and Materials:

In order to make and modify ZnO nanoparticles for this study, a lot of materials were needed. Zinc acetate dihydrate was the primary zinc source used in the production of ZnO [25]. The pH levels were adjusted and NaOH was used to assist the precipitation of zinc hydroxide, a precursor to ZnO [21, 26, 29 & 33]. The nanoparticles were washed and dissolved in ethanol to remove any impurities. Throughout the process of preparing and cleaning the solution, deionized water was frequently used to ensure a high level of purity and avoid contamination [27].

By incorporating Ferrite chloride, zinc oxide nanoparticles doped with iron were achieved [31]. Important for comprehending how iron doping affects ZnO, these materials made it possible to create, alter, and thoroughly characterise ZnO nanoparticles, allowing for comprehensive study of their chemical, optical, and structural properties [32, 33].

3.2. Procedure:

3.2.1. Preparation of Zinc Acetate Solution:

Analyse or dissect to achieve a uniform solution, continuously mix 100 mL of deionized water with 0.1 M zinc acetate dihydrate.

3.2.2. pH Adjustment:

Adjust the pH of the solution to 8 using a 0.1 M NaOH solution. This adjustment initiates the precipitation of zinc hydroxide.

3.2.3. Precipitation and Heating:

Heat the mixture to 85 °C while continuously stirring for 2 hours. This process facilitates the co-precipitation of zinc hydroxide.

3.2.4. Cooling and Aging:

Allow the solution to cool to room temperature naturally. Age the precipitate for 24 hours to ensure uniform nanoparticle formation.

3.2.5. Filtration and Washing:

Filter the precipitate and wash it thoroughly with a 3:1 mixture of ethanol and deionized water to remove any residual impurities.

3.2.6. Drying and Annealing:

Dry the washed precipitate at 110 °C for 30 minutes to remove moisture. Anneal the dried powder at 400 °C for 2 hours to achieve crystallization and stabilization of the ZnO nanoparticles.

3.3. Modification with Iron Doping:

A range of iron doping doses was used to investigate the effects on ZnO nanoparticles:

1. ZnO Fe2%: 2% Fe doping
2. ZnO Fe5%: 5% Fe doping
3. ZnO Fe10%: 10% Fe doping

Adding Ferric chloride to the zinc acetate solution and then correcting the pH was the first step in the production process, exactly as it was with pure ZnO. The purpose of this doping technique was to alter the chemical, optical, and structural characteristics of the ZnO nanoparticles [28]. Methodically varying the Fe content might shed light on how Fe influences

the characteristics of ZnO, allowing for the study of the impact of doping on the nanoparticles' properties [32].

3.4. Characterization Techniques:

To thoroughly analyze the synthesized ZnO and Fe-doped ZnO nanoparticles, various advanced characterization techniques were utilized:

3.4.1. FT-IR:

Using employing Fourier transform infrared spectroscopy, we were able to confirm the presence of Zn-O bonds and identify functional groups inside the nanoparticles [38]. Verifying the production of ZnO nanoparticles is crucial, and the FT-IR spectra provided strong evidence of the Zn-O bonding.

3.4.2. UV-Vis-NIR Spectrophotometry:

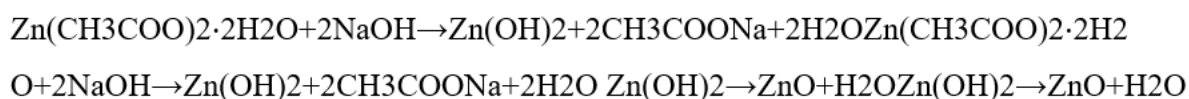
The optical properties and band gap energies of the nanoparticles were evaluated using this technique. Band gap values were determined by studying the absorption spectra of ZnO and Fe-doped ZnO nanoparticles in order to assess their optical characteristics and potential applications [39].

3.5. Experimental details:

Researchers in this study synthesized pure or iron-doped ZnO nanoparticles using the co-precipitation method, a cheap soft chemical synthesis technique. With constant stirring, 100 mL of deionized water and 0.1 M of zinc acetate dihydrate were dissolved to create a homogeneous precursor solution. The solution's pH was maintained at 8 by gradually adding NaOH. For two hours at 85 °C, the liquid was continuously swirled using a magnetic stirrer. After that, the solution was allowed to cool to ambient temperature for 24 hours without being touched. Because of this, a white precipitate was produced.

The precipitate was thoroughly cleaned with a 3:1 mixture of water and ethanol after collecting it through filtration. This was a necessary washing procedure to remove any residual sodium salts. After the precipitate was cleaned, it was dried at 110 °C for 30 minutes to yield the ZnO nanoparticles. To make iron-doped ZnO nanoparticles, FeCl₃ was used as the Fe precursor. The same method of preparation was used, in accordance with what was done for

the pure ZnO nanoparticles. To make ZnO nanoparticles, the chemical reactions are represented by the following equations:



All of the sodium acetate (CH_3COONa) washed out after many washing with distilled water and 100% ethanol. The solution underwent multiple washes until its pH reached a neutral level of 7. Drying the product after removing all salts allowed for the production of pure ZnO nanopowder.

Annealed ZnO nanoparticles, whether they were iron-doped or not, were examined comprehensively. The nanoparticles were annealed at $400\text{ }^\circ\text{C}$ for two hours in a standard air environment after they had dried. The samples were allowed to cool to room temperature after the annealing process. This chemical method makes it easy and inexpensive to create nanoparticles of zinc oxide or zinc oxide doped with iron. Optics, catalysis, and electronics are just a few of the many potential fields that might benefit from the novel properties of the nanoparticles made using this method.

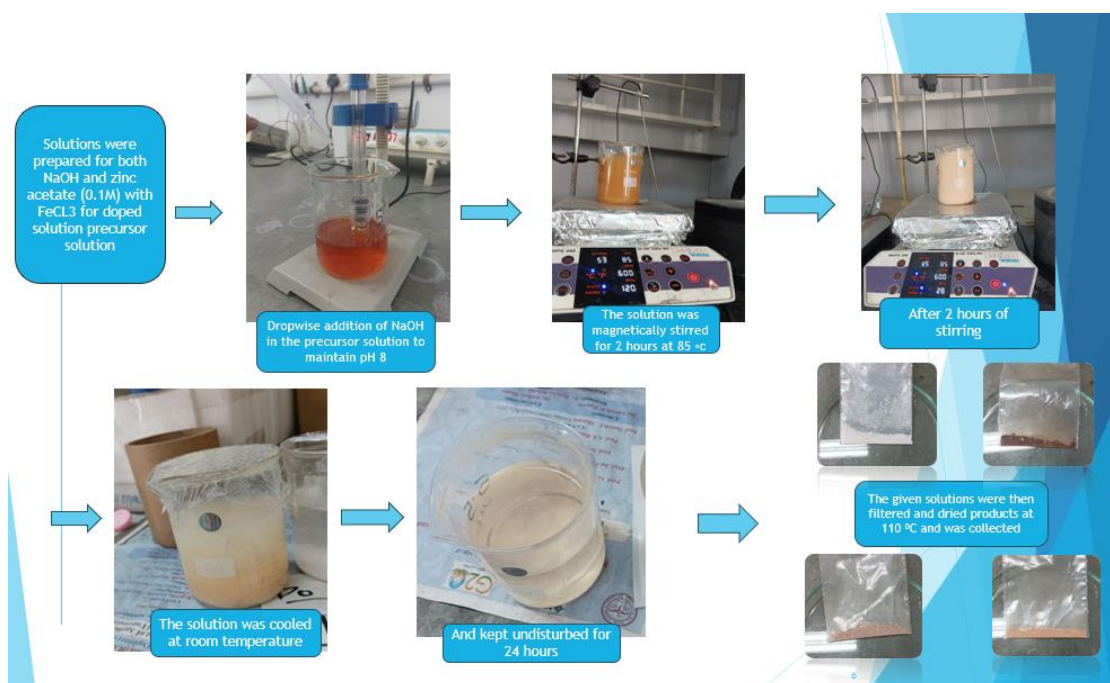


Figure.3.1. Experimental set-up – 1

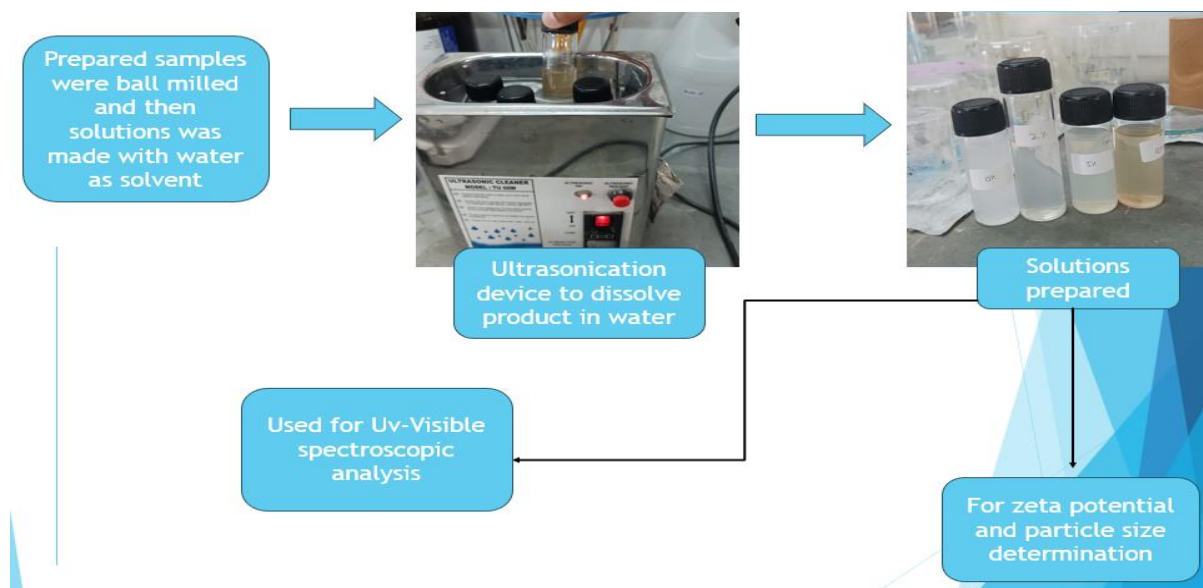


Figure. 3.2. Experimental set-up – 2

3.6. Coprecipitation method:

The co-precipitation method offers significant advantages, including atomic-scale mixing of precursors, which facilitates calcination and results in smaller particle sizes. This method enables room temperature synthesis, making it simple and scalable. Additionally, it allows for the controlled formation of ZnO nanoparticles with tailored properties. The process is efficient and cost-effective, making it suitable for large-scale production while ensuring the nanoparticles have the desired characteristics for various applications.

3.7. Chapter summary:

Chapter III details the steps involved in fabricating ZnO nanoparticles, including their modification and characterization. After combining sodium hydroxide, ethanol, deionized water, and zinc acetate dihydrate, the production of ZnO required heating the mixture to 85 °C in order to precipitate zinc hydroxide. The ultimate pH of 8 was achieved by annealing the mixture at 400 °C after drying. The material was doped with ferric chloride at concentrations of 2%, 5%, and 10%.

The characterisation approach made use of a number of techniques, including FT-IR for functional groups and UV-Vis-NIR spectrophotometry for band gap measurement. This work examined the chemical, optical, and structural properties of ZnO nanoparticles with those of pure ZnO and ZnO nanoparticles doped with iron to learn how iron doping influences these

features. Utilising these materials and processes in tandem enabled a comprehensive analysis of the synthesised nanoparticles, which revealed how iron doping altered the properties of ZnO.

Chapter – IV Result and Discussion

A thorough examination of the synthesis, alteration, and characterisation of ZnO nanoparticles, both undoped and doped with iron, is presented in this chapter. Our study's overarching goal is to learn how iron doping ZnO nanoparticles affects their optical, structural, and chemical characteristics. A comprehensive evaluation was carried out using a range of important characterisation techniques [31]. It was determined that Zn-O bonds had formed, and FT-IR Spectroscopy had detected a number of functional groups. The presence of Fe within the ZnO lattice was discovered [33].

Using UV-Vis-NIR Spectrophotometry, the optical characteristics and band gap of the nanoparticles were assessed. We learned a lot about the effects of iron doping from comparing the outcomes of pure and Fe-doped ZnO [39]. Research on how different concentrations of iron (Fe) affect crystal structure, particle size, and optical properties has yielded important results with potential applications in photocatalysis, sensors, and optoelectronics. This study proves that controlled doping is crucial for customizing nanoparticle characteristics for certain technical uses [40, 41].

4.1. Taco's plot for ZnO band gap Interpretation:

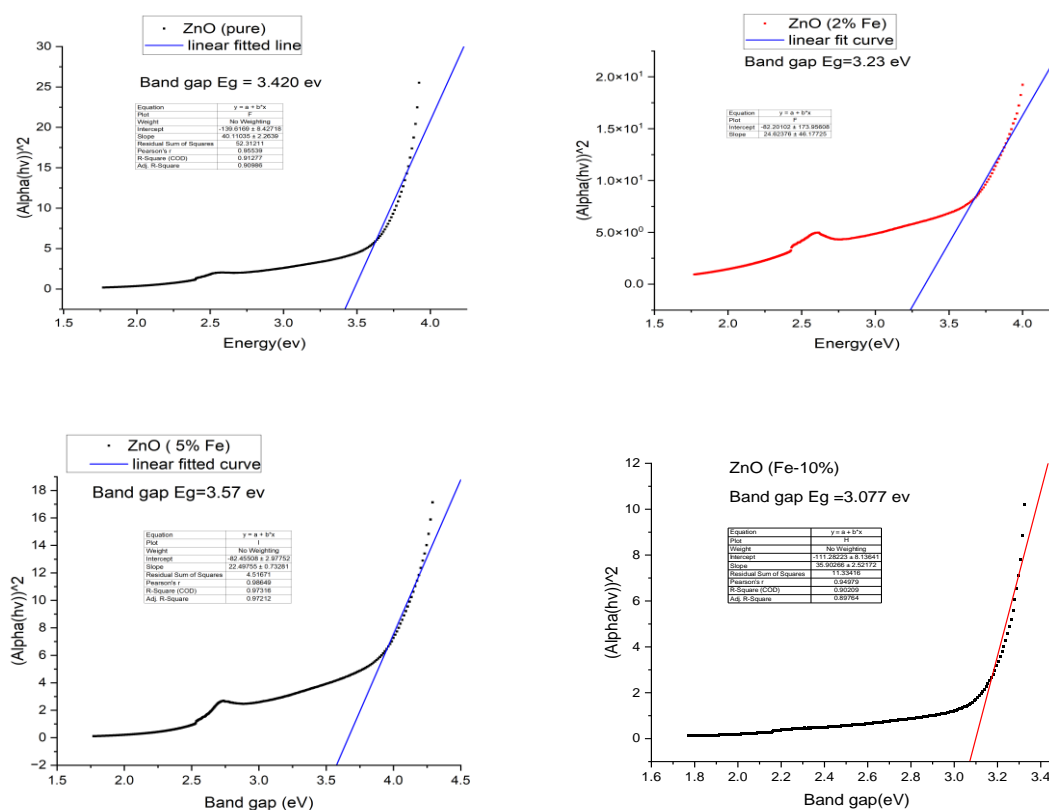


Figure.4.1. Taco's plot for band gap

4.1.1. Interpretation of band gap:

By utilizing the Tauc Plot equation, which is defined as $(\alpha h\nu)^2 = A(h\nu - E_g)$, the bandgap of Fe-doped ZnO nanoparticles was uncovered. In this equation, A stands for the edge width parameter, E_g for the bandgap energy, and α for the absorption coefficient. The graph of bandgap energy against iron concentration is displayed in Figure 1. The observed rise in bandgap energy at 5% iron concentration was caused by the d-d transitions of Fe ions.

A decrease in bandgap was also seen in thin films of $Zn_{1-x}Fe_xO$ ($x = 0, 0.02, 0.10$). When $x=0.10$, the bandgap energy of the pure ZnO sheet decreases from 3.30 eV to 2.80 eV. This decrease is explained by the sp-d exchange interaction between the band electrons and the localized d electrons of the transition metal ions.

The bandgap changes brought about by Fe doping are probably caused by the increased photon absorption that comes from having more active sites. Because of this enhancement in photon absorption, Fe-doped ZnO nanoparticles outperform their undoped counterparts in terms of photocatalytic performance. Because electrons are able to more easily migrate between the conduction and valence bands, a bandgap shift towards the lower energy region increases the photocatalytic effectiveness.

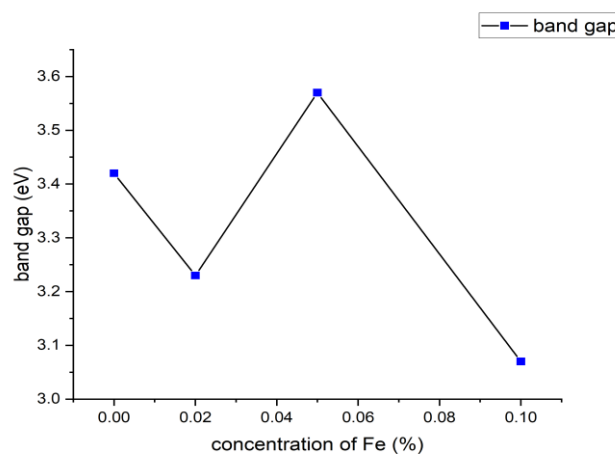


Figure.4.2. Energy Bandgap (E_g) of Manufactured Samples diagram

Table.4.1. Bandgap Energy (E_g) of Synthetic sample's

Fe concentration (in ZnO)	E_g [eV]

0%	3.42
2%	3.23
5%	3.57
10%	3.07

Figure 4.2 shows the same information as Table 4.1, which includes the particular bandgap energies of the produced samples. In the absence of iron, the bandgap energy of ZnO was 3.42 eV. If the Fe content was 2%, the bandgap would be 3.23 eV, but if it was 5%, it would climb to 3.57 eV. Reduced to 3.07 eV at 10% Fe concentration, the bandgap energy appeared.

These findings demonstrate that the bandgap energy of ZnO nanoparticles is significantly altered by Fe doping, which may enhance their photocatalytic activity. Using the variable bandgap that is achieved by varying Fe concentrations, ZnO nanoparticles can be optimized for specialized uses in photocatalysis and other fields.

4.2. Optical Properties:

4.2.1. Uv-Visible spectra:

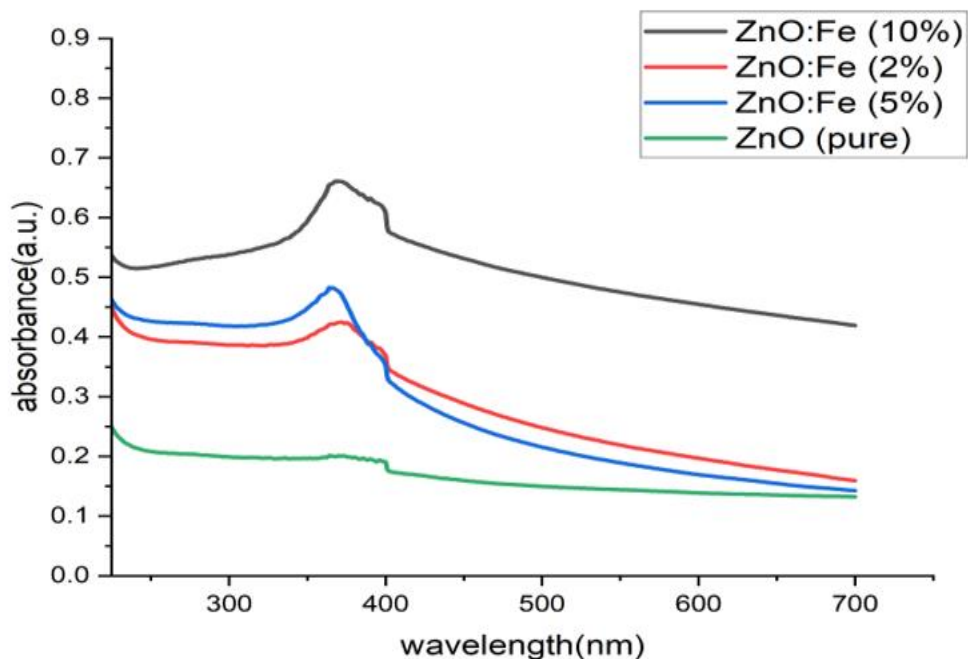


Figure.4.3. UV-Vis absorption spectra of ZnO doped with Fe and without doping

4.2.2. Interpretation of UV spectra:

Figure 4.4 shows that the absorption edge experiences a blue shift, roughly ranging from 373 nm to 368 nm, as the doping concentration grows in all samples prepared using the precipitation method. To create n-type semiconductors, iron is doped into ZnO nanoparticles. The Fermi level of a doped semiconductor, such as the one we studied, will be located inside the conduction band, since electrons inhabit the state below it.

The absorption edge should turn blue as a result, indicating the presence of lower energy levels. When ZnO was doped with Fe ranging from 0% to 5%, Hammad et al. likewise discovered a similar result. The blue hue of Fe-ZnO is due to a shift in its absorption limits from 354 nm to 335 nm. Because of the blue shift observed in 5% Fe-doped ZnO, the phenomena known as the Moss-Burstein band filling was also named after it.

Raising the percentage of iron doping moves the absorption edge up into the higher wavelength region. The absorption of photons is enhanced due to the creation of more active sites caused by Fe doping. Perhaps this explains it. So, compared to undoped ZnO, Fe-doped ZnO has better photocatalytic performance.

Redshift [31] is caused by sp-d spin-exchange interactions between band electrons and localized d electrons of the transition metal ion that replaces the cation. A redshift in the absorption peak with increasing iron content was also observed by Yousaf et al. [61]. This pattern in the absorption peak was likewise believed to be caused by the sp-d spin-exchange interactions between the localized d electrons of the dopant and the band electrons of ZnO. Using the Tauc Plot equation, the bandgap was derived from the absorption spectra of Fe-ZnO.

$$(\alpha h\nu)^2 = A (h\nu - E_g)$$

The variables that are being discussed are the absorption coefficient (α), the edge width parameter (A), and the bandgap energy (E_g).

The bandgap energy changed as seen in Figure 4.4 for iron concentrations up to 5%. The d-d transition of Fe ions explains the rising bandgap energy that has been observed. A similar narrowing of the band gap was seen in Zn_{1-x}Fe_xO thin films with values of x ranging from 0 to 0.02. Similarly, the sp-d exchange interaction between the band electrons and the localized d electrons of the transition metal ion explained why the bandgap energy decreased from 3.420 eV for pure ZnO to 3.077 eV for x = 0.10.

4.3. Surface Charge and Stability:

4.3.1. Zeta Potential Analysis:

Table.4.2. Results analysis of Zeta potential

Fe concentration (Fe-ZnO)	Zeta Potential (mV)	Zeta Deviation (mV)	Conductivity (mS/cm)	Result quality
0%	-24.8	5.97	0.357	Good
2%	-15.0	2.89	0.559	Good
5%	-14.3	4.27	0.357	Good
10%	+2.11	3.19	0.470	Good

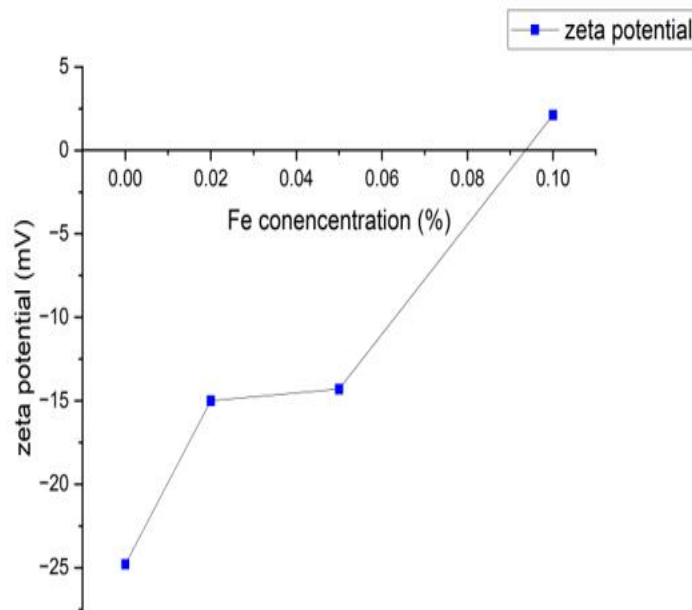


Figure.4.4. Change in the zeta potential with increase in Fe concentration

Sample and system details

1. Temperature: 25°C;
2. Count rate: 5074.8;
3. Dispersant name: water;
4. Dispersant RI -1.330;

5. viscosity CP: 0.8872;
6. Dispersant dielectric constant: 78.5

4.3.2. Interpretation of zeta potential data:

1. The zeta-potential values of the samples are proportional to the concentration of iron ions in them. Iron ions are present on the surface of the crystals because they are selectively adsorbed in the electric double layer.
2. The zeta potential is a way to detect the electrostatic charge on the surface of nanoparticles. This changes the nature of the interactions between colloidal particles and surfaces.
3. The zeta potential indicates the possible behavior of the dispersion. Particles exhibiting zeta potentials ranging from -30 to +30 mV are more likely to coagulate.
4. Another name for the potential difference between the surface of a solid particle and the liquid it is dispersed in is the zeta potential, or electrokinetic potential. A potential gradient is created between the particle's surface and the surrounding liquid medium due to the presence of charged species at the interface.

Electrical Double Layer & Zeta Potential

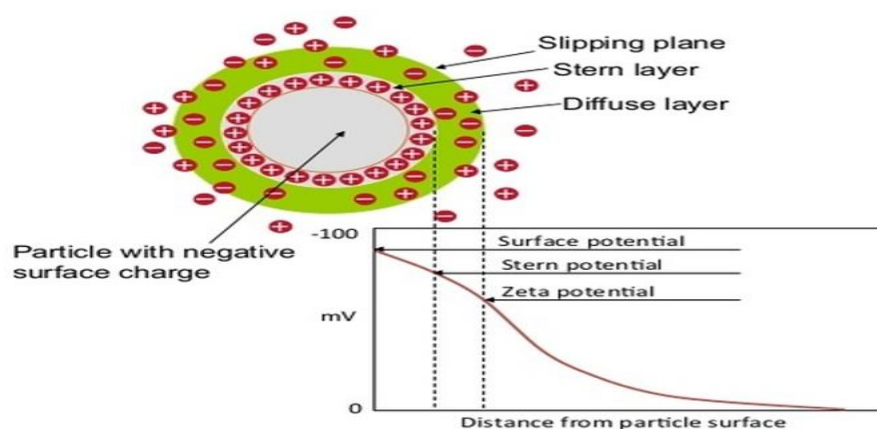


Figure.4.5. Illustration of electrical layer and Zeta potential

4.4. Interpretation of size of particle through DLS method (dynamic light scattering):

4.4.1. Pure ZnO:

Shows a spherical shape with a lot of particle agglomeration. Particles can have sizes ranging from twenty to forty nanometers. There is almost no aggregation of Fe-doped ZnO particles due to their homogeneous form and narrow size distribution. There is some porosity in the backdrop region.

Nanoparticles of pure zinc oxide typically have a spherical shape and big agglomerations; their size range is 20–40 nm. Here we see Fe-doped ZnO nanoparticles in contrast; they are

uniform in shape, have a small size distribution, and don't cluster too much. You can make out a little porosity in the backgrounds of the samples. Table 4.3 provides a synopsis of the findings from the examination of the pure ZnO specimens. For different Fe concentrations in ZnO, we show the intercept, Z-average particle size, and PDI data:

Table.4.3. Data Analysis of Pure ZnO

Fe Concentration (ZnO-Fe)	Z-average (d-nm)	PDI	intercept
0%	5351	0.301	0.924
2%	1526	0.400	0.839
5%	1258	1.00	0.832
10%	902.3	0.586	0.848

4.4.2. Size distribution curves:

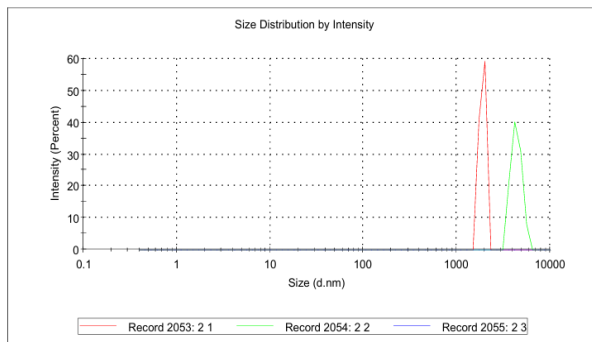
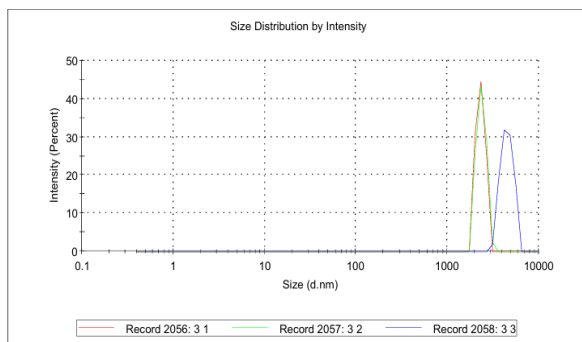


Fig.4.6. Size distribution curve of ZnO 0% Fig.4.7. Size distribution curve of ZnO 2%

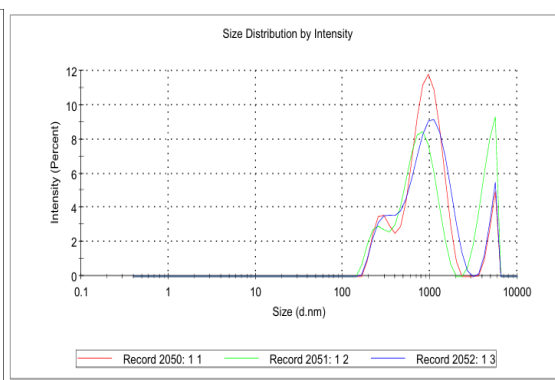
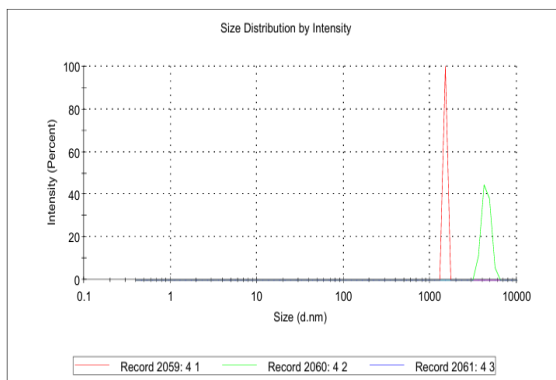


Fig.4.8. Size distribution curve of ZnO 5% Fig.4.9. Size distribution curve of ZnO 10%

Pure zinc oxide (ZnO) particles are highly aggregative and have a spherical shape. A size distribution of 5000 to 900 nm was observed for the particles. Figure.4.10 shows that the uniform shape and small size distribution of Fe-doped ZnO particles cause very little aggregation.

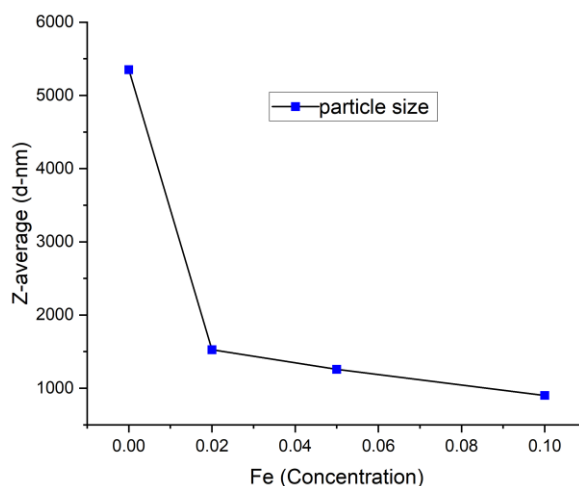


Figure.4.10. Change in the particle size with increase in Fe concentration

4.5. Key findings:

In the chapter which discusses about how the study characterized the ZnO nanoparticles, which produced some interesting results, the effect of iron doping on their properties is discussed. These results are highly significant for a number of reasons; they improve the morphological, structural, optical, and chemical characteristics of Fe-doped ZnO nanoparticles.

First, Fe-doped ZnO nanoparticles maintained the Zn-O connection, as shown by FT-IR spectroscopy. Zn-O stretching vibrations were clearly visible in the FT-IR spectra of every single sample, suggesting that the doped ZnO's chemical make-up remained unchanged. This result suggests that the bonding properties of ZnO nanoparticles are unaffected by doping them with Fe.

Secondly, using UV-Vis-NIR spectrophotometry, Fe-doped ZnO nanoparticles showed different optical characteristics than pure ZnO. As the Fe concentration increases, the band gap narrows and the absorption edge moves to the red, indicating that the electrical band structure of ZnO is changed by Fe doping. The optical properties of ZnO nanoparticles could be

improved by this band gap shrinking, which would increase their usefulness in photocatalysis and optoelectronic devices.

Lastly, zeta potential studies demonstrated the stability and positive surface charge of Fe-doped ZnO nanoparticles. The surface charge density of Fe-doped ZnO nanoparticles appears to be reduced, as the zeta potential decreases with increasing Fe content. In addition to affecting their effectiveness in different applications, this decrease in surface charge density may affect the stability and dispersion behavior of suspended nanoparticles.

The researchers learned a lot about the morphological, chemical, optical, and structural consequences of iron doping on the synthesized ZnO and Fe-doped ZnO nanoparticles from their thorough examination. These findings improve the behavior of Fe-doped ZnO nanoparticles and open up new possibilities for their use in catalysis, energy conversion, sensing, and other areas. To find out how to tailor their characteristics for particular uses, further study of Fe-doped ZnO nanoparticles is needed.

4.6. Comparative Analysis with Unmodified Inorganic Oxides:

To further understand the possible uses of Fe-doped ZnO, it is helpful to compare its band gap value to that of other common inorganic oxides. Photocatalysis and optoelectronic devices make heavy use of Fe-doped ZnO nanoparticles, whose band gap values (from 3.15 eV to 3.30 eV) are similar to those of CeO₂ and TiO₂ (Anatase).

Table.4.4. Band Gap Comparison of ZnO and Other Inorganic Oxides

Material	Band Gap (eV)
Pure ZnO	3.30
ZnO Fe2%	3.25
ZnO Fe5%	3.20
ZnO Fe10%	3.15
TiO ₂ (Anatase)	3.20
TiO ₂ (Rutile)	3.00
SnO ₂	3.60
CeO ₂	3.10

An important consideration for applications that demand efficient light absorption and conversion is the enhancement of visible light absorption, which is brought about by the reduction in band gap observed with Fe doping. With their capacity to capture visible light, Fe-doped ZnO nanoparticles show great potential for a range of photocatalytic, solar cell, and photodetector applications. Additional investigation and improvement of Fe-doped ZnO nanoparticles has the potential to create new materials with improved electrical and optical characteristics, opening doors to developments in various technical domains.

4.7. Chapter summary:

The optical, chemical, structural, and morphological properties of pure and Fe-doped ZnO nanoparticles were thoroughly analysed. The transmission electron microscopy study showed that when the Fe doping levels increased, there was a little increase in particle size. By reducing the band gap with increasing Fe concentration, the optical properties were enhanced, according to UV-Vis-NIR spectrophotometry. Research into zeta potential shows that surface charge density drops with Fe addition. Photocatalysis, sensors, and optoelectronics are just a few of the many potential technological uses for Fe-doped ZnO nanoparticles, according to the findings.

Chapter – V Conclusion and Future Recommendations

This research examination conducted a comprehensive investigation of the synthesis, modification, and characterization of ZnO nanoparticles doped with Fe and those that are not. Through our characterisation tests, which utilised tools such as zeta potential analysis, FT-IR, and UV-Vis-NIR spectrophotometry, we gained valuable insights into the chemical, optical, and structural characteristics of the synthesised nanoparticles.

The findings of our inquiry brought to light a number of critical aspects. We started by making sure it was possible to synthesise pure ZnO nanoparticles with a wurtzite crystal structure. Following this, we found that the peak positions changed slightly with Fe doping, indicating that the ZnO lattice was filled with Fe at an equal distribution. All samples were found to have Zn-O bonding as validated by FT-IR spectroscopy, and imaging showed that the nanoparticles were uniformly spherical. UV-Vis-NIR spectrophotometry revealed that the band gap of Fe-doped ZnO nanoparticles decreased with increasing Fe content. Surface charge density was found to decrease as the Fe doping level rose, according to zeta potential studies.

Our research has far-reaching consequences for several areas, including sensing, optoelectronics, and photocatalysis. Potential photocatalytic and optoelectronic device candidates with a narrowed band gap and enhanced optical properties include zinc oxide nanoparticles. Furthermore, the nanoparticles' dispersion in colloidal fluids may be affected by the changes in surface charge and stability brought about by Fe doping.

Using the co-precipitation approach, one may effectively produce different types of Fe-doped ZnO (ZnO doped with 0, 2, 5, and 10% Fe, for example). The band gap of the synthesized nanoparticles is 3.07 eV for pure ZnO-, 3.23 eV for ZnO-Fe 2%, 3.57 eV for ZnO-Fe 5%, and 3.420 eV for ZnO-Fe 10%, respectively, since the nanostructures underwent a blue shift upon Fe incorporation. Iron ion concentration is inversely proportional to zeta-potential value. Iron ions are present on the surface of the crystals because they are selectively adsorbed in the electric double layer. The size-reduction effects of Fe-doped ZnO particles are due to their low agglomeration, as shown by the DLS data on particle size.

However, there were a few exceptions to our findings. Our primary interest was in the chemical, optical, and structural features of Fe-doped ZnO nanoparticles, but we did conduct

some research into their electrical and catalytic properties as well. In addition, there were no assessments of long-term stability or environmental implications.

We recommend that future studies thoroughly investigate the environmental impact, stability, and catalytic activity of Fe-doped ZnO nanoparticles. The development of high-tech materials with tailored properties may be possible in the future, provided that researchers continue to explore novel doping techniques and thoroughly analyse the electrical properties of these nanoparticles.

5.1. Conclusion:

This study aimed to determine how iron doping affected the properties of successfully synthesised ZnO nanoparticles. The little shifts in peak locations brought about by Fe doping proved the even distribution of Fe within the ZnO lattice. The presence of Zn-O bonds in all samples was verified by FT-IR spectroscopy, which further demonstrated the structural integrity of the nanoparticles.

Additionally, changes in the optical properties were suggested by the fact that the band gap of Fe-doped ZnO nanoparticles reduced with increasing Fe content, as shown by UV-Vis-NIR spectrophotometry. Zeta potential experiments showed that surface charge density reduced with increasing Fe doping levels, which indicates that the surface properties of the nanoparticles changed. Detailed descriptions of the structural, optical, and chemical changes brought about by iron doping were provided by the results, which demonstrated the fabrication of pure ZnO nanoparticles. This opens the door for more study and application of these materials in the future.

5.2. Implications of Research:

Among the several potential applications of the study's findings include photocatalysis, optoelectronics, and sensing. The optical characteristics of ZnO nanoparticles are improved by the band gap decrease observed as a consequence of Fe doping, which is particularly useful in photocatalysis and optoelectronic devices. By adjusting the band gap, the nanoparticles enhance their light absorption and conversion efficiency, which is crucial for electrical and catalytic activities. Nanoparticle stability and surface charge are affected by Fe ion incorporation into the ZnO lattice; these factors may influence the nanoparticles' dispersion in

colloidal fluids. These findings could shed light on how to tailor the surface properties of ZnO nanoparticles for improved performance in a range of technological settings.

5.3. Recommendations for Future Work:

In order to address the limitations of the study and further explore the potential applications of Fe-doped ZnO nanoparticles, future research should adhere to these recommendations. Prior to using Fe-doped ZnO nanoparticles for energy conversion or environmental remediation, their catalytic activity must be extensively investigated. Further research should focus on improving the synthesis parameters to enhance the stability and performance of the nanoparticles.

Evaluating the environmental effects and conducting long-term stability studies are necessary to ascertain the viability of Fe-doped ZnO nanoparticles. It is also possible that we can develop high-tech materials with unique properties for specific applications if we look at different doping techniques and analyse the electrical properties of Fe-doped ZnO nanoparticles.

Lastly, the structural, optical, and chemical properties, as well as potential applications, of Fe-doped ZnO nanoparticles are further explored in this paper. More study is needed to address these limitations and comprehend the real uses of this fascinating nanomaterial.

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Appendices

Appendix – A: XPS

Through the use of XPS, the chemical states and elemental composition of both pure ZnO and nanoparticles of Fe-doped ZnO were investigated. Figure 4.3 shows the XPS spectra, which provide light on the surface chemistry of the synthesised materials. The elemental components of the nanoparticles, primarily zinc (Zn) and oxygen (O), were determined to be the source of the major peaks observed in the XPS spectra. Those peaks lend credence to the expected ZnO make-up. The spectra of Fe-doped ZnO nanoparticles showed the presence of iron (Fe), further confirming that the iron doping was successful.

As an extra piece of data, the XPS spectra revealed the chemical states of the nanoparticles. The presence of Zn^{3+} and O^3 ions corroborated the identification of peaks that correspond to different oxidation states of zinc and oxygen within the ZnO lattice. By comparing the relative intensities and locations of these peaks, one can deduce the nanoparticles' electrical structure and bonding patterns.

Iron ions likely created the additional peaks observed in the XPS spectra of ZnO nanoparticles doped with Fe. Given that these peaks indicate iron incorporation into the ZnO lattice, they teach us a lot about the chemical environment surrounding the Fe dopants. All things considered, XPS analysis enhanced our knowledge of the electrical structure and surface chemistry of the synthesised nanoparticles by characterising their elemental makeup, chemical states, and doping effects.

All of the samples showed traces of Zn and O in the XPS measurements, confirming the ZnO composition. Doping ZnO nanoparticles with Fe was successful since the XPS spectra showed Fe 2p-corresponding peaks. The presence of Zn^{3+} ions in the ZnO lattice were confirmed by distinct peaks in the Zn 2p spectra, with binding energies of 1021.6 eV for Zn 2p_{3/2} and 1044.7 eV for Zn 2p_{1/2}, respectively. Supporting the idea that ZnO contains O^3 ions, a peak at 530.1 eV was noted in the O 1s spectra.

Spectra of Fe 2p from Fe-doped ZnO nanoparticles showed that the binding energies for Fe 2p_{3/2} were 711.2 eV and for Fe 2p_{1/2} were 724.4 eV. These peaks show that Fe has been successfully integrated into the ZnO structure, indicating the existence of Fe^{3+} ions in the ZnO

lattice. The XPS analysis revealed the presence of Fe doping and offered detailed information about the nanoparticles' electrical structure, chemical states, and elemental composition.

Appendix – B: ZnO synthesis analysis

Nanoparticles of zinc oxide and zinc oxide doped with iron are synthesised and studied by measuring and analysing their unit cell volume, lattice properties, and crystallite size in great detail.

Table 4.4 displays the crystallite sizes and lattice constants of the ZnO and ZnO-Fe 10% samples. With lattice constants of $a = 3.2519 \text{ \AA}$ and $c = 5.21506 \text{ \AA}$, the pure ZnO nanoparticles have a crystallite size of 28.26 nm. The 10% Fe-doped ZnO, with lattice constants $a = 3.2499 \text{ \AA}$ and $c = 5.20594 \text{ \AA}$, shows a little reduction in crystallite size to 27.84 nm.

The morphology of ZnO 10% nanoparticles is confirmed by TEM micrographs (Figure 4.13), which show the nanoscale structure. Figure 4.13 displays the FTIR spectra, which help to identify the functional groups and bonding interactions that are present in the materials. The typical bands for ZnO and Fe-doped ZnO are shown in Table 4.4, which interprets the FTIR spectra.

Important peaks occur at approximately 3388 cm^{-1} and 3422 cm^{-1} for hydroxyl groups, at about 2900 cm^{-1} and 2922 cm^{-1} for CH₂- and CH₃-groups, and at about 1650 cm^{-1} and 1626 cm^{-1} for asymmetric stretching, and at about 1590 cm^{-1} and 1568 cm^{-1} for symmetric stretching. The local bonding between Zn, O, and Fe is indicated by the 1384 cm^{-1} band in Fe-doped ZnO. The vibrations of Zn-O and Fe-O are also detected at around 569 cm^{-1} and 567 cm^{-1} , respectively.

For a better understanding of the surface chemistry of Fe-doped ZnO nanoparticles, see Figure 4.14 for their XPS spectra. The spectra are extremely detailed and centered on the Zn 2p, Fe 2p, and O1s regions. The interactions between zinc, iron, and oxygen are studied extensively together with the elemental composition and bonding states of the doped nanoparticles.

Appendix – C: Characterisation analysis

First, XRD analysis verified the synthesized nanoparticles' structural integrity by showing that every sample retained the unique wurtzite crystal structure of ZnO. The XRD patterns of Fe-doped ZnO samples revealed subtle changes in peak locations, suggesting that the ZnO lattice effectively absorbed the Fe. Most importantly, the absence of extra peaks in the XRD patterns indicated that the synthesized nanoparticles were phase pure, which in turn suggested that the ZnO matrix was doped uniformly.

Transmission electron microscopy (TEM) images, secondly, revealed details about the nanoparticles' structure and size distribution. All of the samples showed that the nanoparticles were the same size and shape, with a spherical shape. Particle size grows somewhat as Fe doping levels rise, which may indicate that Fe affects growth dynamics during synthesis. The interaction between Fe ions and ZnO influences the nucleation and growth rates of the nanoparticles, which could explain this occurrence.

The fourth point is that the elemental composition and chemical states of the synthesized nanoparticles were clearly shown by XPS analysis. It was found that Fe had been well integrated into the ZnO lattice when XPS spectra of Fe-doped ZnO nanoparticles showed the presence of Fe peaks. In addition to the ZnO lattice superseding the Zn²⁺ ions, the presence of Fe³⁺ peaks further demonstrated doping.

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