SYNTHESIS AND CHARACTERIZATION OF ZnO-GO NANOPARTICLES FOR PHOTOLUMINESCENCE AND ANTIBACTERIAL APPLICATIONS

PROJECT REPORT

Submitted by

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Submitted to

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In partial fulfillment of the requirements for the award of the degree of

MASTER OF SCIENCE IN PHYSICS

DEPARTMENT OF PHYSICS
ST. TERESA'S COLLEGE (AUTONOMOUS), ERNAKULAM

CERTIFICATE

This is to certify that the project report entitled “**SYNTHESIS AND CHARACTERIZATION OF ZnO-GO NANOPARTICLES FOR THE PHOTOLUMINESCENCE AND ANTIBACTERIAL APPLICATIONS**” is an authentic work done by **TANIYA K C (AM23PHY014)** under my guidance at Department of Physics, St. Teresa’s College (Autonomous), Ernakulam for the partial fulfillment of the requirements for the award of the Degree of Master of Science in Physics during the year 2024-25. The work presented in this dissertation has not been submitted for any other degree in this or any other university.

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M.Sc. PHYSICS

PROJECT REPORT

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Year of Work : **2024-2025**

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DATE:

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DECLARATION

I, TANIYA K C, final year MSc. Physics student of the Department of Physics and Centre for Research, St. Teresa's College (Autonomous), Ernakulam, do hereby declare that the project report entitled "**SYNTHESIS AND CHARACTERIZATION OF ZnO-GO NANOPARTICLES FOR THE PHOTOLUMINESCENCE AND ANTIBACTERIAL APPLICATIONS**" has been originally carried out under the guidance and supervision of **Dr. PRIYA PARVATHI AMEENA JOSE** and **Dr. MARIYAM THOMAS,** Assistant Professors, Department of Physics, St. Teresa's College (Autonomous), Ernakulam in partial fulfilment for the award of the Degree of Master of Physics. I further declare that this project is not partially or wholly submitted for any other purpose and the data included in this project is collected from various sources and are true to the best of my knowledge.

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SYNTHESIS AND CHARACTERIZATION OF ZnO-GO NANOPARTICLES FOR PHOTOLUMINESCENCE AND ANTIBACTERIAL APPLICATIONS

ABSTRACT

Zinc Oxide-Graphene Oxide (ZnO-GO) nanoparticles have garnered considerable attention due to their combined advantageous properties for diverse technological and environmental applications. An incorporation of Zinc Oxide (ZnO) and Graphene Oxide (GO) into its nanoparticles helped in the exploration of various potential properties in optical and antimicrobial activity. In this study, ZnO was synthesized using the sol-gel method with Zinc Acetate and Sodium Hydroxide, while GO was prepared via Hummers' method. ZnO-GO nanoparticles were synthesized by mixing them at appropriate temperatures and they were fabricated at various concentrations 0.5%, 0.75%, and 1 wt%. Structural characterization using X-ray diffraction (XRD) confirmed the formation of ZnO-GO particle, while Fourier-transform infrared spectroscopy (FTIR) verified the presence of functional groups. Optical properties analysed through UV-visible spectroscopy and photoluminescence (PL) studies demonstrated modifications in the electronic structure upon GO incorporation. Antibacterial studies indicated that ZnO-GO nanoparticles displayed enhanced antibacterial activity relative to pure ZnO, emphasizing the synergistic effects between ZnO and GO. The study underscores the potential of ZnO-GO nanoparticles as scalable, multifunctional solutions addressing critical challenges in environmental remediation, energy technology, and healthcare.

Contents

CHAPTER 1

1.1. GENERAL INTRODUCTION

The rapid advancements in material science have propelled researchers to develop novel materials with unique properties for diverse applications, from environmental remediation to advanced electronics. Zinc Oxide (ZnO) and Graphene Oxide (GO) stand out for their exceptional multifunctionality. ZnO, a wide-bandgap (~3.37 eV) semiconductor with high exciton binding energy (~60 meV), is widely utilized in optical applications, sensors, and photocatalysis due to its transparency, conductivity, piezoelectricity, and antibacterial activity. GO, a chemically modified Graphene derivative, features Oxygen-rich functional groups (hydroxyl, epoxy, carbonyl, carboxyl), granting it high hydrophilicity, mechanical strength, tunable electrical properties, and biocompatibility, making it valuable for composites, water purification, biomedical applications, energy storage, and electronics.

A humble attempt was made to synthesize ZnO-GO nanoparticles, as it integrates ZnO's advantages with GO to enhance structural, optical and mechanical properties. Uniform ZnO dispersion on GO improves charge separation, increases active sites, and enhances photocatalytic performance and mechanical stability. These hybrids show superior efficacy in environmental remediation (notably wastewater treatment), energy storage (supercapacitors, lithium-ion batteries), gas sensing, catalysis, biomedical applications, and flexible optoelectronics.

Using robust, scalable methods like sol-gel and modified Hummer's method, ZnO, GO, and ZnO-GO nanoparticles are synthesized and characterized via X-ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), UV-visible spectroscopy, and Photoluminescence Spectroscopy to analyse structural and optical properties. Their antibacterial efficacy is also assessed, demonstrating promising biomedical potential. The outcomes of this research highlight the enhanced capabilities of ZnO-GO nanoparticles, suggesting their promise as multifunctional materials for addressing critical technological and environmental challenges.

1.2. ZINC OXIDE (ZnO)

1.2.1. STRUCTURE OF ZINC OXIDE (ZnO)

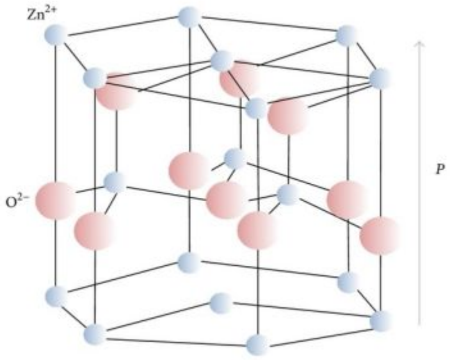


Fig 1.1 Unit Cell of ZnO

Zinc Oxide (ZnO) is a versatile material with a well-defined crystalline structure that significantly influences its properties and applications. Under standard conditions, ZnO predominantly crystallizes in the **wurtzite structure**, a hexagonal close-packed arrangement. This structure is characterized by a unit cell with lattice constants of approximately a = 3.25 Å and c = 5.2 Å, resulting in a c/a ratio close to 1.60, which is slightly less than the ideal ratio of 1.633 for hexagonal systems. The wurtzite structure is thermodynamically stable at room temperature and is the most common form of ZnO used in various applications.

Every Zinc ion (Zn^{2+}) in the wurtzite structure of Zinc Oxide (ZnO) is tetrahedrally bonded to four Oxygen ions (O^{2-}), creating a network of ZnO tetrahedra that share corners. The piezoelectric and pyroelectric properties of ZnO are determined by its tetrahedral coordination and the lack of inversion symmetry of its crystal structure. ZnO's surface reactivity and light-interaction capabilities are further enhanced by the polarity along the c-axis, which is brought about by alternating planes of negatively charged Oxygen ions and positively charged Zinc ions. Because of these special structural characteristics, ZnO is ideal for use in optoelectronics, photocatalysis, sensors, and actuators.

Structure	Description	Key Features
Wurtzite	The most stable structure of ZnO at ambient conditions.	Hexagonal lattice with tetrahedral coordination; commonly used in various applications.
Zincblende	A cubic structure stabilized by growing ZnO epitaxially on cubic substrates.	Features tetrahedral coordination within a cubic lattice; studied for electronic properties in thin films.
Rocksalt	A structure ZnO transitions to under high pressures (above 10 GPa).	Octahedral coordination for Zn and O ions; primarily studied for high-pressure behaviour.

Table 1.1 Structures of ZnO

1.2.2. PROPERTIES OF ZINC OXIDE (ZnO)

a. WIDE BAND GAP

Zinc Oxide (ZnO) is a wide band gap semiconductor (~3.37 eV) with direct band transition, permitting efficient emission and absorption of UV light. In contrast to indirect band gap materials (such as silicon), ZnO does not need phonon assistance for electron movement and consequently is very efficient in optoelectronic devices such as UV lasers, LEDs, and photodetectors. 3.37 eV band gap refers to ~368 nm UV radiation, enabling ZnO to get rid of UV radiation that harms it while continuing to be clear to visible radiation, making ZnO suitable for transparent conductive films and protection against UV rays. The broad band gap increases the thermal and chemical stability of ZnO, making it suitable for use in high-temperature and harsh conditions. It also reduces electron-hole recombination, increasing efficiency in photodetectors, solar cells, and photocatalysis for environmental cleaning. All these make ZnO a universal material for electronic and environmental applications.

b. HIGH EXCITON BINDING ENERGY

Zinc Oxide (ZnO) possesses a large exciton binding energy of approximately 60 meV, which is much larger than many semiconductors such as Gallium Nitride (GaN, approximately 25 meV). Exciton binding energy is the energy to separate an exciton into free carriers. As room-temperature thermal energy is roughly 25 meV, excitons in most material types easily dissociate. ZnO's binding energy is so high, however, that the exciton is stable at room conditions, facilitating intense excitonic emission in the UV range. This makes ZnO a top choice for applications in optoelectronics including UV LEDs, laser diodes, and photodetectors, where strong and efficient luminescence of UV is demanded. This property also favours sophisticated excitonic applications, including polariton lasers, which utilize excitons for effective light amplification. Exciton-dominated behaviour improves UV luminescence and quantum confinement effects in ZnO nanostructures such as nanorods and nanowires, making them extremely useful for nanoscale optoelectronic devices. ZnO's stable UV emission also has biomedical uses, including fluorescence-based biosensors and high-resolution imaging, where sharp and consistent emissions are essential.

c. TRANSPARENCY AND CONDUCTIVITY

Zinc Oxide (ZnO) exhibits high transparency to visible light coupled with tunable n-type conductivity, making it crucial for optoelectronics. Its broad band gap of 3.37 eV precludes absorption of visible light (1.65–3.1 eV), while its high optical clarity is critical for transparent conductive oxides (TCOs) in touchscreens, displays, and solar cells. ZnO is also transparent to the near-UV range, rendering it suitable for UV-absorbing but optically transparent applications. Besides, its capacity to produce uniform films provides uniform transparency on large industrial devices. ZnO's inherent n-type conductivity is the result of intrinsic defects such as Oxygen vacancies, supplemented by doping with materials like aluminium (Al), Gallium (Ga), or Indium (In) to enhance conductivity while maintaining transparency. This make ability enables ZnO to function as a transparent electrode in solar cells, with charge transport promoted without blocking light. Its cost-effectiveness, abundance, and ease of processing make ZnO a good candidate to replace indium Tin Oxide (ITO) in current optoelectronics, adding strength to its position in high-performance displays, touchscreens, and energy-saving devices.

Property	Applications	Key Notes
UV Light Emission	Used in light-emitting diodes (LEDs) and UV lasers for efficient charge transport and optical clarity.	Doped ZnO ensures performance in UV-emitting devices while maintaining transparency.
Sensors	Transparent conductive layers in sensors respond to environmental changes, like gas concentrations or temperature.	Suitable for gas sensing and environmental monitoring applications.
Smart Windows	ZnO films regulate light transmission and heat exchange in energy-efficient building designs.	Contributes to sustainable and energy-efficient technologies.

Table 1.2 Conductivity Applications of ZnO

d. PIEZOELECTRICITY

Zinc Oxide (ZnO) exhibits **piezoelectric properties** due to its unique **non-centrosymmetric crystal structure**. Piezoelectricity is the ability of certain materials to generate an electric charge in response to applied mechanical stress or, conversely, to undergo mechanical deformation when subjected to an electric field. This dual functionality is a direct result of the atomic arrangement in ZnO's crystalline lattice, making it a valuable material in various mechanical-electrical energy conversion applications.

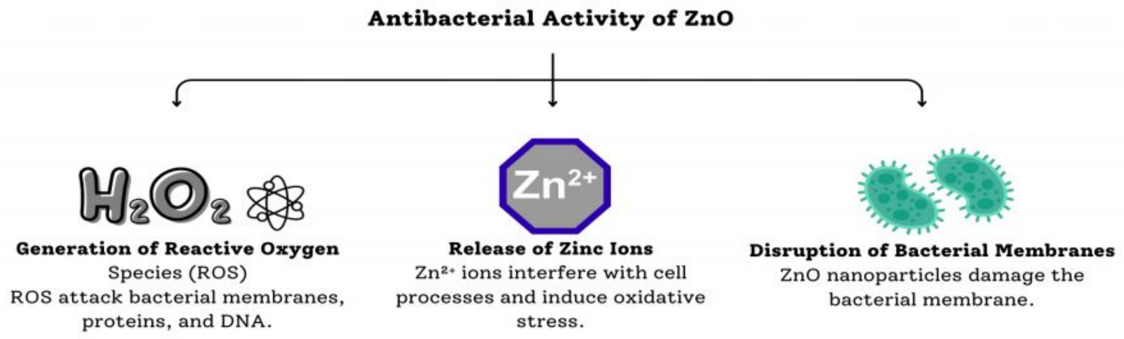
The wurtzite structure of ZnO that lacks inversion symmetry, where Zinc and Oxygen ions are positioned in tetrahedral coordination along the polar c-axis and when a mechanical stress is applied along this axis, it causes a distortion in the crystal lattice, resulting in a separation of positive and negative charges. This separation creates an electric dipole, which generates a measurable electric potential across the material. The piezoelectric effect of ZnO is particularly strong due to its high ionic bonding character, which increases the displacement of ions when mechanical stress is applied and therefore this property makes ZnO one of the most effective piezoelectric materials among semiconductors, especially in its nanoscale forms like nanowires and nanorods.

Application	Description	Examples/Uses
Energy Harvesting	Converts mechanical energy into electrical energy using ZnO nanogenerators.	Wearable devices, sensors, and LEDs.
Sensors and Actuators	Detects pressure/strain or converts electrical signals to mechanical motion.	Robotics, MEMS, and industrial machinery.
Biomedical Applications	Used in biosensors and implantable devices for biomolecular detection and biological monitoring.	Enzyme/DNA biosensors, implantable devices.
Acoustic Devices	Generates acoustic waves for signal processing in SAW devices.	Telecommunications and environmental sensing.
Vibration Sensors	Detects mechanical vibrations for accelerometers and structural health monitoring.	Automotive and aerospace engineering.

Table 1.3 Piezoelectric Applications of ZnO

e. ANTIBACTERIAL ACTIVITY

Zinc Oxide (ZnO) is widely recognized for its **antibacterial properties**, which make it a valuable material in medical, environmental, and industrial applications. The antibacterial effects of ZnO stem from its ability to generate reactive Oxygen species (ROS), its direct interaction with bacterial membranes, and its release of Zinc ions, which disrupt cellular processes.



ROS attack bacterial membranes, proteins, and DNA.

Zn^{2+} ions interfere with cell processes and induce oxidative stress.

ZnO nanoparticles damage the bacterial membrane.

Fig 1.2 Antibacterial Activity of ZnO

Some advantages of ZnO as an antibacterial agent are as follows:

- **Broad-Spectrum Activity:** ZnO is effective against a wide range of microorganisms, including gram-positive and gram-negative bacteria, as well as some fungi and viruses. This broad-spectrum activity makes ZnO suitable for diverse antibacterial applications.
- **Biocompatibility:** ZnO is considered biocompatible, meaning it is safe for use in medical applications such as wound dressings, coatings for surgical instruments, and drug delivery systems.
- **Resistance to Antibiotic Resistance:** Unlike traditional antibiotics, ZnO's physical and oxidative mechanisms of action make it less likely to induce bacterial resistance, addressing a critical issue in healthcare.
- **UV Activation for Enhanced Activity:** The antibacterial effects of ZnO can be significantly enhanced under UV light due to increased ROS generation. This property is particularly useful in applications requiring sterilization, such as in water purification systems.

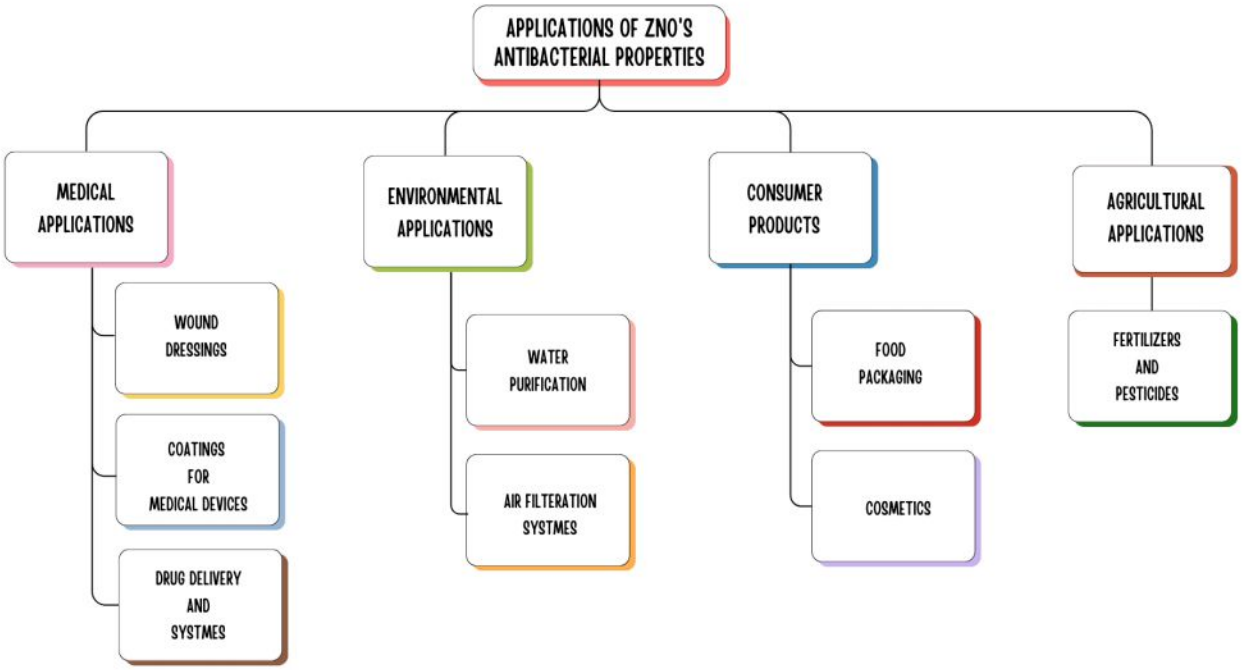


Fig 1.3 Applications of ZnO’s Antibacterial Properties

1.3. GRAPHENE OXIDE (GO)

1.3.1. STRUCTURE OF GRAPHENE OXIDE (GO)

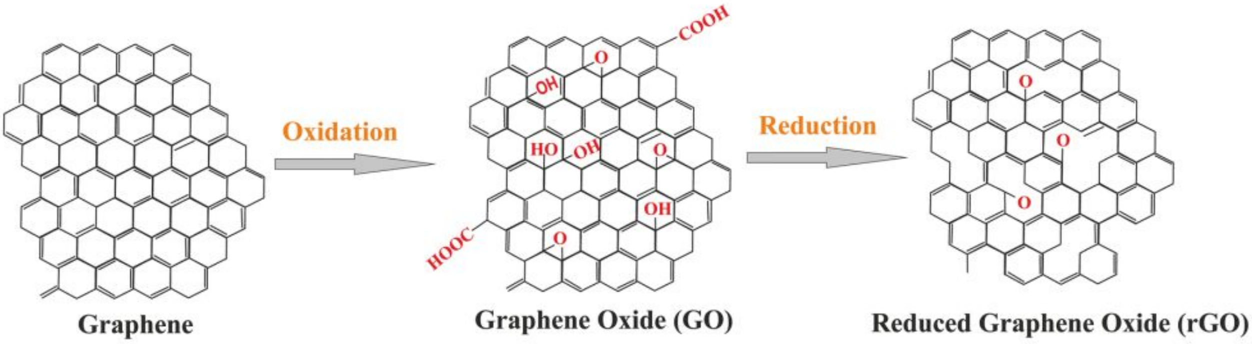


Fig 1.4 Molecular Structure of Graphene, Graphene Oxide, Reduced Graphene Oxide

Graphene Oxide (GO) is a two-dimensional, single-atomic-layer material derived from graphite through chemical oxidation and exfoliation. Its structure can be thought of as a modified Graphene sheet, decorated with a variety of Oxygen-containing functional groups. These functional groups, which include hydroxyl (-OH), epoxy (C–O–C), carbonyl (C=O), and carboxyl (-COOH) groups, are distributed on both the basal plane and the edges of the GO sheet. This functionalization significantly alters the properties of GO compared to pristine Graphene, introducing hydrophilicity, chemical versatility, and a disrupted electronic structure.

The basal plane of Graphene Oxide (GO) is primarily composed of hydroxyl and epoxy groups, disrupting the sp^2-hybridized carbon lattice and creating sp^3-hybridized regions, which reduces electrical conductivity but enhances chemical reactivity. The edges of GO contain carboxyl and carbonyl groups, which are vital for functionalization and interfacial interactions with other materials. These functional groups impart a non-uniform structure, providing a combination of sp^2 and sp^3 areas, which provides GO partial conductivity, high surface area, and chemical tunability. GO also has a layered structure, with larger interlayer distance (0.6–1.2 nm vs. 0.34 nm in graphite), facilitating ion and molecule diffusion between layers. This feature makes GO a good candidate for applications in membranes, adsorbents, and energy storage devices.

Functional Group	Location	Description
Epoxy Groups ($C–O–C$)	Basal plane	Contribute to structural disruption, reducing electrical conductivity.
Hydroxyl Groups ($–OH$)	Basal plane	Enhance hydrophilicity, enabling dispersion in water and polar solvents.
Carboxyl Groups ($–COOH$)	Edges of GO	Increase chemical reactivity and facilitate covalent bonding with other materials.
Carbonyl Groups ($C=O$)	Edges of GO	Contribute to reactivity and functionalization potential.

Table 1.4 Functions Groups of GO

The introduction of these functional groups disrupts the sp^2 hybridization of the Graphene lattice, introducing sp^3 hybridized regions. This modification reduces the electrical conductivity of GO compared to Graphene but enhances its chemical versatility and solubility in water.

Graphene Oxide (GO) has a disordered structure due to the introduction of Oxygen groups, which distort its hexagonal symmetry and create defects, giving it semiconducting or insulating properties depending on oxidation levels. Some of the conductivity is restored through partial reduction to reduced Graphene Oxide (rGO). GO is structurally heterogeneous, with varying oxidation levels and functional group distributions, which affect its performance in different applications. Despite this, GO retains a high surface area (0.8–1.2 nm thickness for a monolayer), offering numerous active sites for adsorption, chemical reactions, and composite formation, making it useful in water purification, catalysis, and energy storage.

Structural Characteristic	Description
Chemical Reactivity	Highly reactive due to functional groups on basal plane and edges.
Mechanical Strength	Retains strength due to carbon backbone, ideal for composites.
Thermal Stability	Stable up to 200°C; decomposes and partially reduces beyond that.

Table 1.5 Impact of GO on certain properties

1.3.2. PROPERTIES OF GRAPHENE OXIDE (GO)

a. HIGH SURFACE AREA

Graphene Oxide (GO) is a two-dimensional (2D) material known for its incredibly high surface area, thanks to its single-atomic-layer thickness and large lateral dimensions. This unique characteristic, combined with the presence of Oxygen-containing functional groups like hydroxyl, carboxyl, and epoxy, makes GO particularly effective in adsorption tasks, such as removing heavy metals, dyes, and organic pollutants for water purification and environmental cleanup. In the fields of catalysis and photocatalysis, GO helps prevent the clumping of catalysts, enhances charge separation, and boosts the degradation of pollutants and Hydrogen production, making it essential for various catalytic processes. Additionally, GO enhances composite materials by improving their mechanical, thermal, and electrical properties. When added to polymers, ceramics, or metals, it strengthens interfacial bonding, leading to better structural integrity. In energy storage applications, GO's extensive surface area allows for efficient charge transport and storage, which significantly enhances the performance of supercapacitors and lithium-ion batteries. These qualities position GO as a highly versatile material for advanced functional uses.

b. HYDROPHILICITY

Graphene Oxide (GO) is extremely hydrophilic because of Oxygen-containing functional groups (hydroxyl, carboxyl, epoxy, and carbonyl) that are distributed along its basal plane and edges. These functional groups provide strong affinity toward water molecules so that GO can develop stable colloidal suspensions in polar solvents—opposite to Graphene, which is predominantly hydrophobic. Such hydrophilicity is vital in solution-based processing for ease of manipulation, functionalization, and deposition onto substrates. It facilitates clean production of thin films, coatings, and electrically conductive materials for the electronics industry alongside improved accuracy in 3D printing and inkjet printing operations.

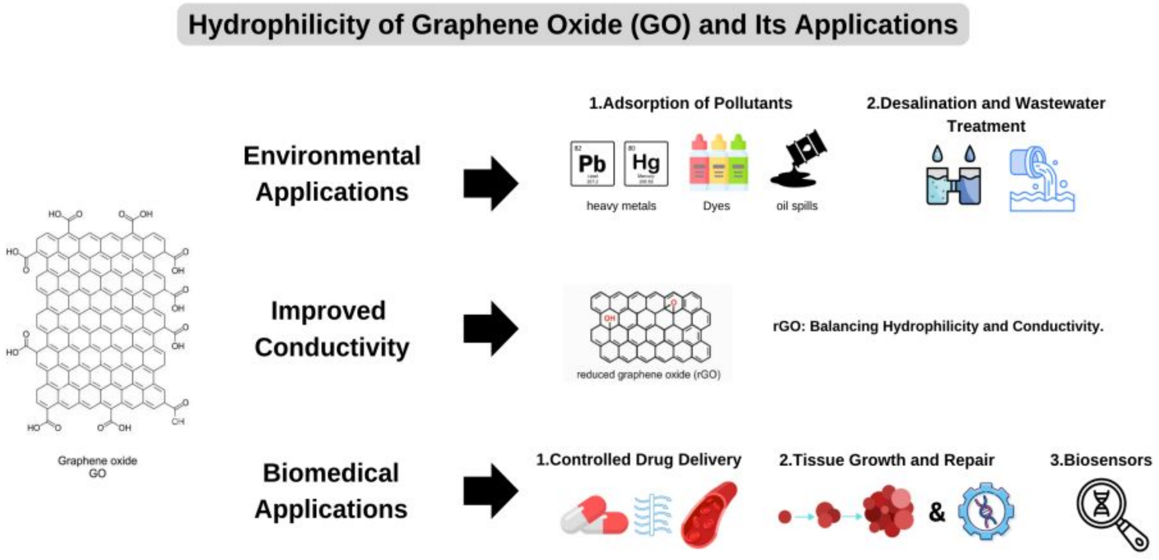


Fig 1.5 Hydrophilic Applications of GO

c. CHEMICAL VERSATILITY

Graphene Oxide (GO) is very versatile because its Oxygen-containing functional groups (hydroxyl, carboxyl, epoxy, and carbonyl) allow covalent and non-covalent functionalization. Covalent modifications are through strong chemical bonds like amide formation between the carboxyl group and amines or reaction with hydroxyl and epoxy groups. These facilitate GO to incorporate into polymers, biomolecules, and nanoparticles to improve mechanical, thermal, and electronic properties. Conversely, non-covalent interactions maintain the structure of GO but allow for reversible modification towards applications such as sensors, drug delivery, and catalysis.

GO's chemical flexibility also renders it a superior composite material, reinforcing polymers, ceramics, and metals and enhancing conductivity, thermal stability, and toughness. Functionalized derivatives of GO can be designed to fit specific applications, like metal-nanoparticle hybrids for catalysis or organic-functionalized GO for biomedicine. GO's tunable surface chemistry renders it a critical material in high-technology applications, such as water purification, energy storage, and high-performance coatings.

d. BIOCOMPATIBILITY

Graphene Oxide (GO) is extremely biocompatible and has the potential to be used as a drug delivery material, in tissue engineering, biosensing, and regenerative medicine. GO's hydrophilicity provides stability in biological fluids, avoids aggregation, and allows for controlled drug release through covalent or non-covalent interactions. GO has a high surface area and facilitates high drug-loading capacity, improving therapeutic efficacy with reduced side effects. In tissue engineering, it enhances scaffold bioactivity, supporting cell adhesion, proliferation, and differentiation, and increases mechanical stability in hydrogels and biomaterials. GO also enhances biosensor sensitivity by increasing sensitivity and specificity in diagnostics. But its concentration and formulation need to be optimized to avoid oxidative stress or inflammation. Research targets surface modifications, for example, biopolymer coatings and biocompatible functionalization, aimed at improving safety while maintaining its useful properties, rendering GO a multi-purpose material for the next generation of healthcare technologies.

e. TUNABLE ELECTRICAL PROPERTIES

Graphene Oxide (GO) has tunable electrical properties because it can be reduced chemically, thermally, or electrochemically to reduced Graphene Oxide (rGO). Oxygen functional groups break GO's sp^2 hybridized carbon network, decreasing conductivity. Controlled reduction treatments eliminate these groups, restoring part of the sp^2 network and enhancing electrical conductivity. By controlling the level of reduction, GO and rGO can be optimized for electronics, energy storage, and sensor applications where conductivity needs to be controlled with precision.

Application	Key Features
Electronic Devices	rGO serves as a cost-effective alternative to Graphene, enabling its use in flexible circuits, transparent conductive films, and field-effect transistors (FETs). Simplified fabrication processes allow large-scale manufacturing.
Energy Storage	rGO is used in supercapacitors as an electrode material due to its high surface area, conductivity, and charge storage capacity. In lithium-ion batteries, it acts as an anode material, enhancing charge transport, energy density, and cycling stability.
Sensors	GO is highly sensitive for detecting chemical and biological analytes. rGO improves conductivity while retaining functional groups, enhancing performance in gas, biomolecule, and pollutant sensors.

Table 1.6 Tunable Electric Applications of GO

f. MECHANICAL STRENGTH

Graphene Oxide (GO) is known for its impressive mechanical strength, even when its structure is compromised by oxidation. Although the presence of functional groups diminishes its intrinsic strength compared to pure Graphene (approximately 1 TPa), GO still maintains a high Young’s modulus ranging from 200 to 250 GPa, which is greater than that of most traditional materials. Its two-dimensional layered structure, combined with strong covalent bonds, makes it an outstanding reinforcement material, significantly boosting the mechanical properties of polymers, ceramics, and metals. In composite materials, GO enhances stress transfer through effective interfacial bonding, leading to improvements in tensile strength, elasticity, and toughness. The layered “brick-and-mortar” structure of GO also helps to dissipate energy, which prevents crack propagation and increases fracture toughness, especially in brittle ceramic composites.

The functional groups present in GO allow for compatibility and chemical modifications, which enable the creation of customized composites with enhanced mechanical, thermal, and chemical properties. In metal matrix composites, GO contributes to increased strength and wear resistance, making it ideal for high-stress applications. Additionally, GO-based thin films and coatings provide high tensile strength and flexibility, making them suitable for applications in flexible electronics, protective coatings, and filtration membranes. To optimize the performance of GO, factors such as the degree of oxidation, sheet size, and dispersion quality must be carefully managed, with ongoing research focused on refining synthesis and functionalization techniques to maximize strength while preserving desirable characteristics.

1.3.3. APPLICATIONS OF GRAPHENE OXIDE (GO)

Graphene Oxide (GO) is a versatile material with exceptional properties that make it suitable for a wide range of applications. Its unique combination of high surface area, functional group diversity, and mechanical strength underpins its effectiveness in industries such as water purification, energy storage, composite materials, biomedicine, and electronics. Below is a detailed exploration of its key applications.

a. WATER PURIFICATION

Graphene Oxide (GO) is very efficient in water purification because of its high surface area and rich functional groups, which facilitate adsorption of heavy metals, dyes, and organic pollutants via ion exchange and complexation. Its capacity to remove contaminants even at trace levels makes it suitable for wastewater treatment and environmental remediation. GO-based membranes have high selectivity and permeability, effectively filtering salts, organic molecules, and pathogens and are thus of great use in desalination and advanced water treatment. GO also improves photocatalytic degradation when used with catalysts such as ZnO or TiO_2, facilitating the degradation of recalcitrant pollutants and pathogens under light irradiation. This synergy is a sustainable and energy-efficient means of water purification.

b. ENERGY STORAGE

Graphene Oxide (GO) is essential in energy storage systems because of its large surface area, chemical stability, and adjustable electrical properties. In supercapacitors, GO boosts charge storage by utilizing electrical double-layer capacitance and pseudo capacitance, which creates numerous active sites for ion adsorption, thereby enhancing energy density and cycle life. In lithium-ion batteries, GO acts as an anode material or electrode component, improving conductivity, charge transport, and structural integrity during charge-discharge cycles. Furthermore, GO enhances ion exchange and durability in fuel cells, aiding in the creation of efficient and long-lasting energy conversion devices.

c. COMPOSITES

Graphene Oxide (GO) significantly improves composite materials by boosting their mechanical strength, thermal stability, and electrical conductivity. In polymer composites, GO strengthens the matrix by forming strong interfacial bonds, which enhances load transfer and resistance to mechanical stress. This makes it particularly suitable for structural materials, protective coatings, and flexible electronics. In metal and ceramic composites, GO enhances toughness, reduces brittleness, and improves fracture resistance, making these materials ideal for high-performance aerospace and automotive applications. Furthermore, GO enhances wear resistance and thermal stability in metal composites, thereby extending their lifespan in challenging environments.

d. BIOMEDICAL APPLICATIONS

Graphene Oxide (GO) is extremely biocompatible and functionally diverse, which makes it suitable for biomedical applications. In drug delivery, its functional groups allow for targeted and controlled release of therapeutic molecules, minimizing side effects and maximizing treatment efficacy. Its large surface area also enhances drug-loading capacity, making it useful in cancer therapy and other treatments. In tissue engineering, GO-based scaffolds facilitate cell adhesion, proliferation, and differentiation, supporting tissue regeneration. In addition, functionalized GO improves biosensors for the detection of biomolecules such as glucose, DNA, and proteins with high sensitivity to serve disease diagnostics, environmental monitoring, and personalized medicine.

e. ELECTRONICS AND SENSORS

In the field of electronics, GO is used to develop flexible and transparent devices. GO-based conductive films are utilized in touchscreens, wearable electronics, and transparent electrodes. Their high conductivity, combined with their flexibility, makes them ideal for next-generation devices that require lightweight, bendable components. Furthermore, GO's sensitivity to gases such as CO_2, NH_3, and volatile organic compounds is leveraged in the development of high-performance gas sensors. These sensors are widely applied in environmental monitoring, industrial safety, and healthcare.

f. CATALYSIS AND PHOTOCATALYSIS

GO is an excellent support material for catalysts, improving their dispersion, stability, and overall activity. Its large surface area ensures uniform distribution of catalyst particles, preventing agglomeration and maximizing active sites. In photocatalytic applications, GO enhances light absorption and charge transfer when combined with semiconductors like ZnO and TiO_2. This synergy accelerates pollutant degradation under light irradiation, making GO-based photocatalysts valuable for environmental remediation and clean energy production.

1.4. ZnO-GO NANOPARTICLES

1.4.1. STRUCTURE OF ZnO-GO NANOPARTICLES

ZnO-GO nanoparticles combine Zinc Oxide (ZnO) nanoparticles with Graphene Oxide (GO) sheets to form a hybrid material with improved properties for future applications. ZnO, in nanoparticle, nanorod, or nanowire forms, offers high surface area and active sites for catalysis, sensing, and energy storage, while its semiconducting and photocatalytic nature allows for effective electron-hole generation. GO, with its Oxygen-containing functional groups and two-dimensional structure, guarantees strong interaction with ZnO, leading to uniform dispersion, hindering aggregation, and facilitating charge separation for higher efficiency.

The hybrid adopts a "brick-and-mortar" architecture with GO as an elastic matrix, and the addition of ZnO provides functionality and stiffness. The architecture enhances interfacial adhesion, charge transfer, and the suppression of electron-hole recombination, while advancing photocatalytic and electric properties. The coupling of ZnO's high reactivity with GO's high surface area places ZnO-GO nanoparticles well-suited for water purification, energy storage, and environmental remediation, drawing on ZnO's photocatalytic activity and GO's conductivity to achieve optimal performance in next-generation technologies.

1.4.2. PROPERTIES OF ZnO-GO NANOPARTICLES

a. ENHANCED PHOTOCATALYTIC ACTIVITY

The ZnO-GO nanoparticle shows improved photocatalytic activity thanks to the synergistic interaction between Zinc Oxide (ZnO) and Graphene Oxide (GO). ZnO absorbs UV light, creating electron-hole pairs that initiate redox reactions, leading to the production of reactive Oxygen species (ROS) for degrading pollutants and splitting water. However, the rapid recombination of electron-hole pairs limits the efficiency of ZnO. GO helps to overcome this issue by serving as an electron acceptor, which enhances charge separation and electron mobility, thereby significantly boosting quantum efficiency. GO's large surface area and functional groups improve the adsorption of pollutants, while its close contact with ZnO creates a heterojunction that promotes efficient charge transfer. This heterojunction mechanism helps to prevent recombination and maximizes photocatalytic efficiency. Furthermore, the uniform dispersion of ZnO on GO optimizes light absorption and catalytic interactions, making ZnO-GO nanoparticles particularly effective for environmental remediation and energy applications.

Application	Description	Key Benefits
Wastewater Treatment	Degradation of organic pollutants like dyes and pesticides.	Ensures complete mineralization into non-toxic byproducts (water and CO_2) through ROS generation.
Air Purification	Removal of volatile organic compounds (VOCs) and other airborne pollutants.	ROS effectively degrade airborne pollutants, improving air quality.
Photocatalytic Water Splitting	Hydrogen generation through enhanced charge separation.	Facilitates the Hydrogen evolution reaction (HER), supporting clean energy production.
Water Disinfection	Destruction of harmful microorganisms, including bacteria and viruses.	ROS eliminate pathogens, ensuring safe and clean water.

Table 1.7 Photocatalytic Environmental Applications of ZnO-GO Nanoparticles

b. IMPROVED ELECTRICAL CONDUCTIVITY

The ZnO-GO nanoparticle shows much higher electrical conductivity compared to pure Zinc Oxide (ZnO) because of the synergistic interaction between ZnO and Graphene Oxide (GO). Although ZnO's wide bandgap restricts its conductivity, GO serves as a good electron transporter with enhanced charge transfer and minimized resistive losses. The partially retained sp^2-hybridized carbon domains of GO allow electron transport, particularly after reduction to rGO, forming conductive channels that enhance the electric performance of the composite. On the ZnO-GO interface, GO acts as an electron reservoir, transferring photoexcited electrons from ZnO quickly, diminishing recombination, and extending the availability of charge. Uniform deposition of ZnO onto GO optimizes the transfer of charges, and interfacial anchoring through the functional groups in GO ensures solid structural stability. These factors increase the efficacy of ZnO-GO immensely towards energy storage applications, where optimized conductivity raises the capacitance value in supercapacitors and improves the cycle stability of lithium-ion batteries. Furthermore, in sensors, the high conductivity of the composite enhances sensitivity and response time, whereas in optoelectronics, it allows for lightweight, transparent conductive films for displays, touch screens, and solar cells, guaranteeing optimal efficiency and performance.

c. HIGH SURFACE AREA

Large surface area of ZnO-GO nanoparticles improves their performance in catalysis, energy storage, and environmental remediation. This is due to the synergistic interaction between GO's 2D planar structure and ZnO's nanostructured morphology, forming a hybrid material with high activity sites for chemical interactions. GO's Oxygen functional groups enhance adsorption and dispersion of uniform ZnO, inhibiting aggregation and enhancing surface-driven processes. Nanostructured forms of ZnO further amplify the surface-to-volume ratio, improving reactivity and stability along with the advantage of GO's structural support.

In photocatalysis, improved surface area enhances light absorption and pollutant interaction, while effective charge transfer from ZnO to GO enhances photocatalytic efficiency. In energy storage, it offers sufficient sites for ion adsorption and charge transport, increasing capacitance in supercapacitors and charge-discharge stability in lithium-ion batteries. For ecological use, the large surface area of the composite facilitates adsorption of pollutants and ZnO allows for photocatalytic degradation, which makes it extremely useful for water treatment and air purification.

d. MECHANICAL AND THERMAL STABILITY

The ZnO-GO nanoparticle has superior thermal and mechanical stability because of the synergy between ZnO's thermal stability and GO's mechanical strength. The 2D nature of GO, high aspect ratio, and strong covalent bonds toughen the composite, while its functional groups provide strong interfacial interactions with ZnO. This hinders ZnO agglomeration and creates a "brick-and-mortar" structure wherein GO is flexible and ZnO makes it rigid. The outcome is a very resistant material that can bear mechanical stresses, and thus it is applicable in flexible electronics, coatings, and structures. The inbuilt thermal stability of ZnO, in combination with the thermal dissipation capacity and prevention of particle detaching of GO, keeps the composite functional at high temperatures. Strong interfacial bonding of GO with ZnO avoids high-temperature degradation by minimizing local thermal stress. Due to this, ZnO-GO nanoparticles find applications at high temperatures in the form of catalytic converters, sensors, and electronic components where thermal durability and long-term performance are demanded.

Application	Overview	Key Benefits
Flexible Electronics	Ability to endure repeated bending and deformation without losing structural integrity.	Ensures durability and consistent performance in flexible electronic devices.
High-Temperature Catalysis	Delivers consistent results under extreme thermal conditions for reactions like pollutant degradation and fuel processing.	Maintains efficiency and stability in high-temperature environments.
Protective Coatings	Withstands harsh environments, ideal for machinery, pipelines, and aerospace components.	Enhances durability and protection against wear, corrosion, and extreme conditions.
Energy Devices	Efficient operation in batteries and supercapacitors under high current loads generating heat.	Ensures thermal stability and long-term performance for energy storage systems.

Table 1.8 Mechanical and Thermal Applications of ZnO-GO Nanoparticles

e. VERSATILE FUNCTIONALIZATION

The multi-faceted functionalization of ZnO-GO nanoparticles is due to the Oxygen-containing functional groups of Graphene Oxide (GO) and the chemical reactivity of Zinc Oxide (ZnO), which enables controlled modifications for various applications. GO's hydroxyl, carboxyl, epoxy, and carbonyl groups enable strong covalent and non-covalent bonding with ZnO, providing structural stability and the ability for further chemical modifications. Covalent bonding permits the attachment of catalysts, biomolecules, or polymers, whereas non-covalent interactions like van der Waals forces and Hydrogen bonding facilitate reversible functionalization, rendering the composite flexible for dynamic applications such as sensors and drug delivery. ZnO in the composite can also be metal-doped (e.g., silver, iron, cobalt) to develop photocatalytic, antibacterial, or electronic performance. Such versatility allows ZnO-GO composites to dominate water purification through pollutant adsorption and catalysed degradation, energy storage through charge transport optimization, biomedicine through drug delivery and biosensing, and catalysis through metal nanoparticle or enzyme support. The capacity to tune the chemical, mechanical, optical, and electrical properties of the composite makes it a versatile material for sophisticated technological applications.

1.4.3. APPLICATIONS OF ZnO-GO NANOPARTICLES

ZnO-GO nanoparticles are versatile materials with enhanced properties that make them suitable for a wide range of applications. The synergy between Zinc Oxide (ZnO) and Graphene Oxide (GO) enables superior performance in water purification, energy storage, gas sensing, catalysis, biomedical applications, and optoelectronics. Below is a detailed exploration of these applications.

a. WATER PURIFICATION

ZnO-GO nanoparticles are highly effective in water purification due to their combined photocatalytic and adsorption capabilities. In photocatalysis, ZnO acts as the primary catalyst, generating reactive Oxygen species (ROS) such as hydroxyl radicals (•OH) under UV or visible light. These ROS degrade organic pollutants, including dyes and pesticides, into non-toxic byproducts. GO enhances this process by acting as an electron acceptor and transporter, reducing the recombination of photogenerated electron-hole pairs in ZnO. This improves the efficiency of pollutant degradation, making the composite suitable for wastewater treatment and environmental remediation. In addition to photocatalysis, GO's functional groups and layered structure enable the composite to adsorb a wide range of contaminants, such as heavy metals (e.g., lead and mercury), organic pollutants, and pathogens. The adsorption process is facilitated by the high surface area and chemical affinity of GO, which capture contaminants efficiently. Together, the photocatalytic activity of ZnO and the adsorption properties of GO make the composite an excellent material for water purification, addressing both chemical and biological pollution.

b. ENERGY STORAGE

ZnO-GO nanoparticles are widely used in energy storage devices due to their high surface area, conductivity, and electrochemical activity. In supercapacitors, the composite serves as an electrode material with enhanced charge storage capacity and stability. GO contributes to the composite's conductivity and provides a large surface area for ion adsorption, while ZnO offers electrochemical activity, facilitating redox reactions. This combination results in high capacitance and excellent cycling stability, making the composite ideal for advanced energy storage systems. In lithium-ion batteries, ZnO-GO nanoparticles function as high-performance anode materials. The composite structure ensures efficient charge transport and storage by leveraging GO's conductivity and ZnO's ability to intercalate lithium ions. The uniform dispersion of ZnO on GO prevents agglomeration, ensuring structural stability during repeated charge-discharge cycles. This synergy leads to improved energy density, cycling stability, and rate performance, making ZnO-GO composites a promising material for next-generation batteries.

c. GAS SENSING

The ZnO-GO composite exhibits high sensitivity and selectivity for gas sensing applications. ZnO, as a semiconducting material, responds to gas molecules by altering its electrical conductivity, a property that is enhanced by the presence of GO. GO's large surface area provides abundant active sites for gas adsorption, improving sensor response and sensitivity. The combination of ZnO's semiconducting nature and GO's conductivity allows for faster electron transfer, ensuring quick detection of gases such as ammonia, Carbon Dioxide, and volatile organic compounds (VOCs). The composite's ability to detect gases at low concentrations makes it suitable for environmental monitoring, industrial safety, and healthcare applications. For instance, ZnO-GO-based sensors can be used to monitor air quality, detect toxic gas leaks, or measure metabolic gases in medical diagnostics.

d. CATALYSIS

ZnO-GO nanoparticles are highly effective in photocatalysis and electrocatalysis due to their synergistic properties. In photocatalysis, ZnO absorbs light to generate electron-hole pairs, while GO enhances charge separation and transport, improving efficiency in water splitting for Hydrogen generation and pollutant degradation in environmental applications. In electrocatalysis, ZnO-GO materials catalyse reactions like Oxygen reduction and Hydrogen evolution, where GO's functional groups and ZnO's active sites enhance reaction rates and stability. With high surface area and conductivity, the composite is well-suited for fuel cells, electrochemical sensors, and other energy-related applications.

e. BIOMEDICAL APPLICATIONS

The biocompatibility and functional versatility of ZnO-GO nanoparticles make them suitable for biomedical applications. In drug delivery, the composite's functional groups enable the attachment and transport of therapeutic molecules. GO provides a large surface area for drug loading, while ZnO's biocompatibility ensures safe interaction with biological systems. This allows for controlled and targeted drug release, minimizing side effects and improving treatment efficacy. ZnO-GO nanoparticles are also used as antimicrobial coatings for medical devices and surfaces. ZnO's antibacterial properties, combined with GO's biocompatibility, create a composite that can effectively prevent bacterial growth and biofilm formation. These coatings are particularly useful in surgical instruments, implants, and wound dressings, where infection control is critical.

f. OPTOELECTRONICS

In optoelectronic applications, ZnO-GO nanoparticles are used in devices such as UV photodetectors, light-emitting diodes (LEDs), and transparent conductive films. ZnO's wide bandgap and high exciton binding energy make it an excellent material for UV light detection and emission, while GO provides flexibility and enhanced charge transport. The combination of these properties results in improved device performance, such as higher sensitivity in photodetectors and increased efficiency in LEDs. The flexibility and transparency of GO also make the composite suitable for transparent conductive films used in touchscreens, displays, and solar cells. These films leverage GO's mechanical strength and ZnO's optoelectronic properties to create lightweight, durable, and efficient devices for modern electronics.

1.4.4. KEY ADVANTAGES OF ZnO-GO NANOPARTICLES

Leveraging the strengths of both Zinc Oxide (ZnO) and Graphene Oxide (GO), these nanoparticles exhibit enhanced functionality, scalability, and adaptability, making them suitable for a wide range of advanced applications. Below is a detailed exploration of these key advantages.

Key Advantage	Description	Applications
Synergistic Performance	Combines the best properties of ZnO (photocatalysis, semiconducting, piezoelectricity) and GO (conductivity, versatility).	Enhanced photocatalysis, energy storage, sensors, and optoelectronics.
Scalability	Easily synthesized using cost-effective, large-scale methods like hydrothermal synthesis and sol-gel processes.	Industrial applications in environmental remediation, energy storage, and healthcare.
Versatility	Tailorable composite by adjusting ZnO: GO ratio or functionalizing components with catalysts, biomolecules, or polymers.	Flexible electronics, conductive films, catalysis, biomedicine, and environmental applications.

Table 1.9 Advantages of ZnO-GO Nanoparticles

1.5. LITERATURE SURVEY

1.5.1. ZINC OXIDE (ZnO)

Klingshirn (2007) provided a comprehensive review of the fundamental properties of ZnO, emphasizing its significance as a wide-bandgap semiconductor with a direct bandgap of approximately 3.37 eV. This property enables ZnO to absorb and emit ultraviolet (UV) light efficiently, making it an essential material for UV photodetectors and light-emitting diodes (LEDs). Additionally, ZnO exhibits a high exciton binding energy of 60 meV, which allows excitons to remain stable at room temperature, further enhancing its UV luminescence efficiency. The structural stability and chemical robustness of ZnO enable its application in high-temperature and corrosive environments, which broadens its scope across various industries.

Willander et al. (2009) highlighted the structural properties of ZnO, specifically its hexagonal wurtzite crystal structure, which contributes to its piezoelectric and ferroelectric properties. These properties make ZnO a versatile material for sensors, actuators, and energy harvesting devices. The study also explored the role of intrinsic defects, such as Oxygen vacancies and Zinc interstitials, in imparting n-type semiconducting behaviour to ZnO. Furthermore, the authors discussed various doping strategies to tune ZnO’s electrical conductivity for advanced applications, such as transistors and gas sensors.

The synthesis of ZnO nanostructures has been extensively studied and optimized using various methods. *Moezzi* et al. (2012) discussed the hydrothermal method as an environmentally friendly approach for synthesizing ZnO nanorods and nanowires with high crystallinity. The sol-gel method, another widely used technique, was noted for its ability to produce ZnO with precise control over size and morphology. Chemical vapor deposition (CVD) has also been employed for the fabrication of ZnO thin films, particularly in optoelectronic applications, due to its ability to produce high-quality layers. Precipitation and electrochemical deposition methods have further enabled scalable and cost-effective synthesis of ZnO for industrial use.

ZnO’s applications are as diverse as its properties. *Wang* et al. (2018) emphasized its role in photocatalysis, where ZnO generates reactive Oxygen species under UV light to degrade organic pollutants effectively. This property is extensively utilized in wastewater treatment and air purification systems. In energy storage, ZnO has demonstrated exceptional performance as an active material in supercapacitors and lithium-ion batteries. The high electrochemical activity and stability of ZnO improve charge storage and cycling performance, making it an indispensable material for next-generation energy storage technologies.

Additionally, ZnO's sensitivity to environmental changes has been leveraged in gas sensing applications. *Djurišić* et al. (2012) highlighted the development of ZnO-based sensors for detecting gases such as ammonia, Hydrogen, and volatile organic compounds. These sensors exhibit high sensitivity and selectivity due to ZnO's semiconducting properties and high surface area. In biomedical applications, ZnO's antibacterial properties and biocompatibility have enabled its use in drug delivery systems, tissue engineering, and antimicrobial coatings. Its piezoelectric properties are further utilized in energy harvesting devices and pressure sensors, highlighting ZnO's multifunctionality.

1.5.2. GRAPHENE OXIDE (GO)

Dreyer et al. (2010) provided a detailed review of the chemistry of Graphene Oxide (GO), highlighting its structural characteristics and chemical versatility. GO is a two-dimensional material derived from graphite through chemical oxidation and exfoliation processes. It consists of a single layer of carbon atoms arranged in a honeycomb lattice, similar to Graphene, but is heavily decorated with Oxygen-containing functional groups such as hydroxyl (-OH), epoxy (C–O–C), carboxyl (-COOH), and carbonyl (C=O) groups. These functional groups disrupt the sp^2-hybridized Graphene lattice, introducing sp^3-hybridized regions that alter its electronic, optical, and mechanical properties. This modification makes GO chemically reactive, hydrophilic, and dispersible in polar solvents, differentiating it significantly from pristine Graphene.

Pei and *Cheng* (2012) discussed the tunable properties of GO, particularly its electrical conductivity, which can be controlled by reducing GO to reduced Graphene Oxide (rGO). The reduction process partially restores the sp^2-conjugated network, enhancing its conductivity while retaining some Oxygen groups for functionalization. This tunability makes GO and rGO versatile materials for applications in electronics, sensors, and energy devices. The study also highlighted that the choice of reduction method—thermal, chemical, or electrochemical—

significantly affects the final properties of rGO, offering a pathway to tailor materials for specific applications.

Singh et al. (2011) emphasized GO's high surface area, which arises from its two-dimensional sheet structure. This feature provides abundant active sites for adsorption and chemical reactions, making GO a highly efficient material for environmental applications such as water purification. GO's functional groups also enable it to adsorb heavy metals, dyes, and organic pollutants, facilitating its use in wastewater treatment. Additionally, the layered structure of GO contributes to its performance in filtration membranes for desalination and advanced purification systems.

Compton and *Nguyen* (2010) discussed the role of GO in composite materials, where its incorporation enhances the mechanical, thermal, and electrical properties of the host material. GO's Oxygen-containing functional groups enable strong interfacial bonding with polymers, metals, and ceramics, resulting in composites with improved performance. For example, GO-reinforced polymer composites exhibit increased tensile strength and thermal stability, making them suitable for structural and high-temperature applications.

In the field of energy storage, *Dreyer* et al. (2010) highlighted the use of GO as an electrode material in supercapacitors and lithium-ion batteries. GO's high surface area and conductivity enable efficient charge storage and transport, improving the energy density and cycling stability of these devices. The study also noted the role of GO in hybrid electrodes, where its synergy with active materials such as metal oxides enhances overall performance.

GO's biocompatibility and functional versatility make it a valuable material in biomedical applications. *Pei* and *Cheng* (2012) discussed its use in drug delivery systems, where the functional groups on GO facilitate the attachment of therapeutic molecules for targeted delivery and controlled release. GO-based scaffolds in tissue engineering promote cell adhesion and proliferation, supporting tissue regeneration. Additionally, GO's optical properties have been leveraged in biosensing and imaging applications, providing high sensitivity and specificity in detecting biomolecules.

1.5.3. ZnO-GO NANOPARTICLES

Wang et al. (2018) conducted a comprehensive study on ZnO-GO nanoparticles, focusing on their synthesis, characterization, and applications. They highlighted that the combination of ZnO and GO results in a hybrid material with enhanced photocatalytic activity, electrical conductivity, and mechanical stability compared to the individual components. The uniform dispersion of ZnO on GO, facilitated by strong interfacial bonding through GO's Oxygen-containing functional groups, plays a crucial role in enhancing these properties. The intimate interaction between ZnO and GO improves charge transfer and reduces electron-hole recombination, making the nanoparticle highly effective for photocatalytic applications.

Zhang et al. (2012) emphasized the role of GO in extending ZnO's photocatalytic response from UV to visible light by facilitating light absorption and charge separation. Their study demonstrated the degradation of organic dyes and pharmaceutical pollutants using ZnO-GO nanoparticles, showcasing the composite's potential in environmental remediation. Additionally, Lv et al. (2013) described the use of hydrothermal and sol-gel methods for synthesizing ZnO-GO composites, highlighting how the synthesis process influences the composite's morphology and performance. The hydrothermal method, in particular, was noted for producing ZnO with uniform dispersion on GO, leading to enhanced photocatalytic efficiency.

In the field of energy storage, ZnO-GO nanoparticles have shown significant promise. *Geng* et al. (2018) reported that the synergy between ZnO's electrochemical activity and GO's high conductivity results in improved performance in supercapacitors and lithium-ion batteries. The incorporation of GO enhances charge transport and cycling stability, while ZnO contributes to the overall energy density. The study further demonstrated the composite's ability to sustain high-performance cycling under repeated charge-discharge conditions, making it suitable for next-generation energy storage systems.

In optoelectronics, *Wang* et al. (2018) demonstrated that the integration of ZnO and GO improves device performance in UV photodetectors and transparent conductive films. The wide bandgap of ZnO, combined with the flexibility and conductivity of GO, creates hybrid materials that are both efficient and mechanically robust. This makes ZnO-GO composites suitable for use in advanced optoelectronic devices.

1.6. OVERVIEW

Zinc Oxide (ZnO) and Graphene Oxide (GO) are versatile materials with unique properties that make them valuable for advanced applications. ZnO, a wide-bandgap semiconductor, exhibits excellent photocatalytic, piezoelectric, and optical properties but suffers from rapid electron-hole recombination and limited conductivity. GO, with its high surface area, tunable conductivity, and functional groups, enhances the performance of ZnO when combined, forming ZnO-GO nanoparticles. This synergy improves charge separation, electrical conductivity, and structural stability, making the composite highly effective in environmental remediation, energy storage, and sensing applications.

This thesis focuses on the synthesis and characterization of ZnO, GO, ZnO-GO nanoparticles. The study investigates their structural and optical properties. Characterization techniques such as XRD, UV and FTIR are employed to analyse the material properties and their influence on functionality. Properties of fluorescence and anti-bacterial activity is also studied. The outcomes demonstrate that ZnO-GO nanoparticle overcome the limitations of pure ZnO, offering enhanced photocatalytic efficiency, improved conductivity, and mechanical stability.

CHAPTER 2

2. EXPERIMENTAL TECHNIQUES

2.1. SYNTHESIS OF ZINC OXIDE (ZnO)

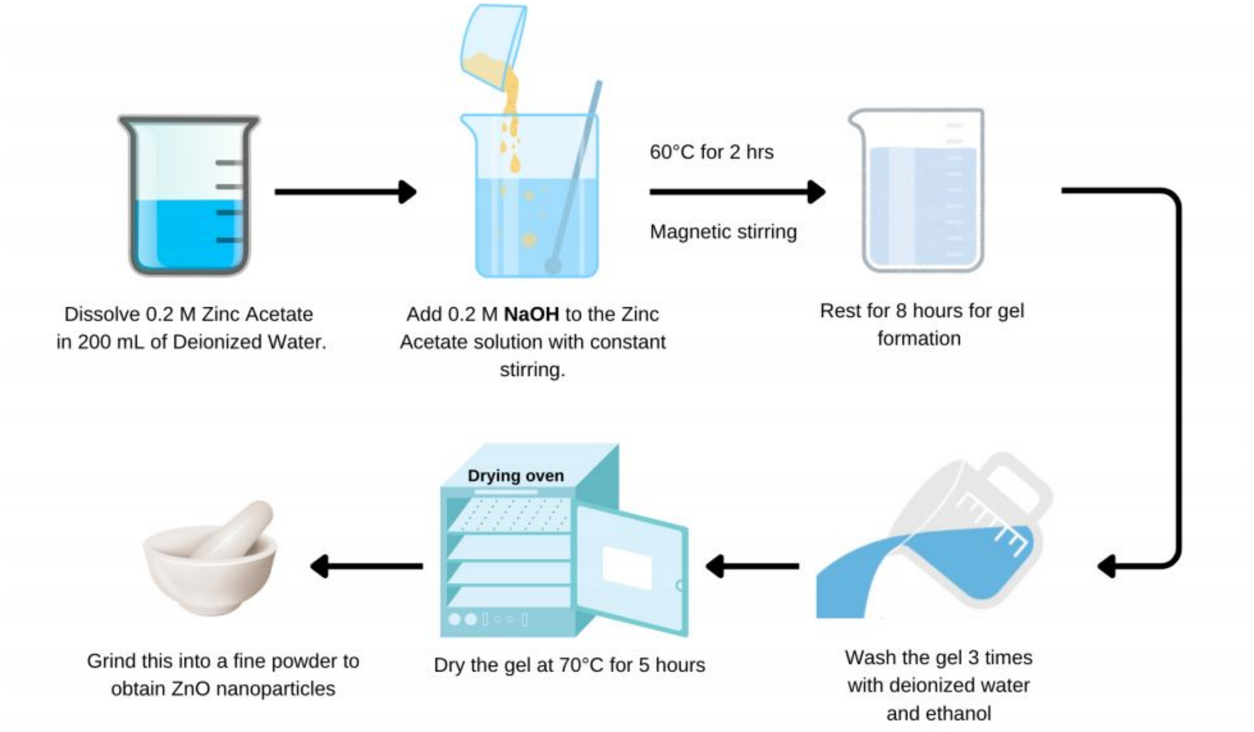


Fig 2.1 Synthesis of ZnO

Zinc Oxide (ZnO) nanoparticles were synthesized via the sol-gel method, a widely used technique for producing nanoparticles with uniform size and high purity. This method leverages the hydrolysis and condensation of precursor materials to form a gel, followed by thermal treatment to yield nanoparticles.

To begin, 0.2 mol of Zinc Acetate dihydrate ($Zn(CH3COO)2 \cdot 2H2O$), a common Zinc precursor, was dissolved in 200 mL of deionized water. The solution was stirred thoroughly to ensure complete dissolution of the precursor, resulting in a homogeneous solution. This step is critical for achieving uniform particle formation in subsequent stages.

Separately, a 0.2 molar solution of Sodium Hydroxide (NaOH) was prepared by dissolving an appropriate amount of NaOH in 200mL volume of deionized water. The NaOH solution was then slowly and carefully poured to the Zinc Acetate solution under continuous stirring to maintain uniform mixing and to avoid localized precipitation. The slow pouring to the Zinc Acetate solution also facilitates controlled pH adjustment, which is essential for forming a stable gel.

The reaction mixture was maintained at 60°C with constant stirring for 2 hours to facilitate the hydrolysis and condensation reactions. These reactions led to the formation of a colloidal solution that began to gelation. The mixture was subsequently allowed to rest undisturbed for 8 hours at room temperature, enabling complete gel formation. This resting period is necessary to achieve structural uniformity and ensure that the gel is well-formed.

The resulting gel was subjected to a purification process to remove any unreacted precursors and by-products. It was washed three times alternately with deionized water and ethanol. Deionized water ensured the removal of soluble impurities, while ethanol helped in eliminating organic residues and enhancing the drying process.

After washing, the purified gel was dried in an oven at 70°C for 5 hours. This drying step removed any remaining moisture, which is critical for preventing agglomeration and maintaining nanoparticle quality. Then calcinated at 400°C for 2 hours. This is essential for crystallization of ZnO. Finally, the dried gel was ground into a fine powder using a ceramic mortar and pestle. This grinding process further improved the uniformity and consistency of the ZnO, preparing them for characterization and various applications.

The sol-gel method employed in this synthesis provides several advantages, such as simplicity, scalability, and the ability to produce nanoparticles with controlled morphology and high purity. The resulting ZnO are well-suited for a range of applications, including photocatalysis, sensors, and biomedical fields, due to their uniform size, enhanced surface area, and superior chemical and physical properties. This synthesis protocol represents a reliable and efficient approach for producing ZnO with reproducible quality for research and industrial purposes.

2.2. SYNTHESIS OF GRAPHENE OXIDE (GO)

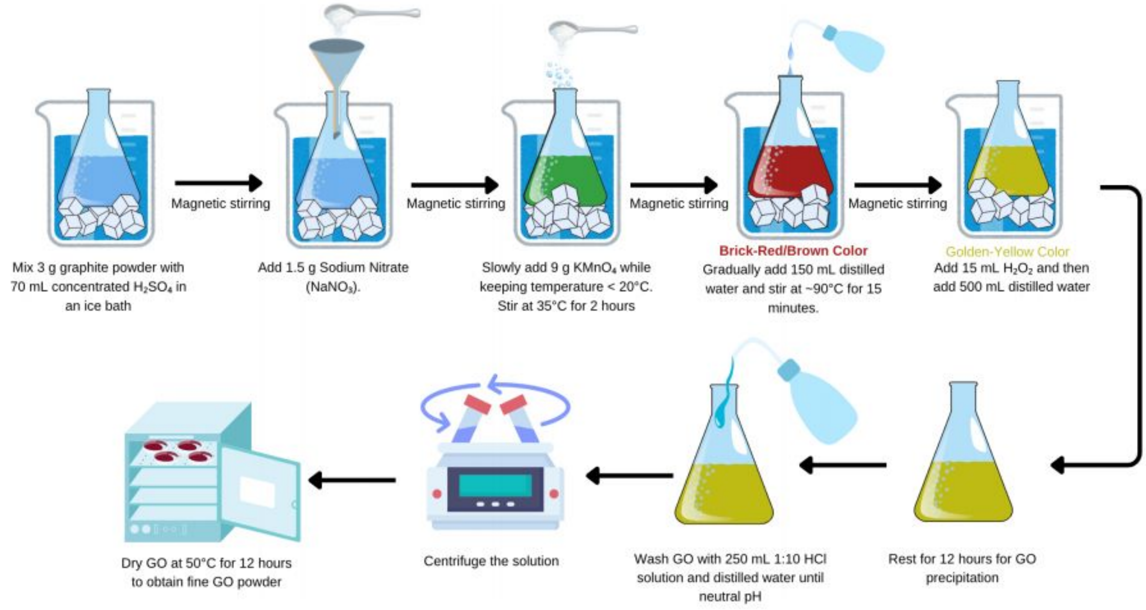


Fig 2.2 Synthesis of GO

Graphene Oxide (GO) was synthesized using the modified Hummer's method, a widely adopted approach for obtaining high-quality GO from graphite. The process involves multiple chemical reactions and purification steps to ensure the complete oxidation of graphite and the removal of impurities, resulting in a pure GO product suitable for various applications.

The preparation began with mixing 3 g of graphite powder with 70 mL of concentrated sulfuric acid (H_2SO_4) while maintaining the reaction mixture in an ice bath to control the temperature. This step ensures safe handling of the exothermic reaction in subsequent additions. Once the graphite was uniformly dispersed in the acid, 1.5 g of Sodium Nitrate ($NaNO_3$) was added under continuous stirring to further activate the graphite and aid the oxidation process.

Next, 9 g of Potassium Permanganate ($KMnO_4$) was slowly introduced to the reaction mixture while maintaining the temperature below 20°C to avoid excessive heat generation and ensure safety. The slow addition of $KMnO_4$ initiated the oxidation process, turning Graphite into Graphite Oxide. The mixture was then stirred at a slightly elevated temperature of 35 ± 5°C for 2 hours to allow the oxidation to proceed effectively.

Afterward, the thick solution was gradually diluted by adding 150 mL of distilled water under continuous stirring. This dilution step was performed carefully to prevent rapid heat generation due to the exothermic nature of the reaction. The solution was further stirred at approximately 90°C for 15 minutes, enhancing the reaction and ensuring complete oxidation of graphite.

To neutralize excess permanganate and Manganese ions, 500 mL of additional distilled water was added to the mixture, followed by the slow addition of 15 mL of Hydrogen Peroxide (H_2O_2). This step resulted in a visible colour change, indicating the formation of Graphene Oxide. The resulting suspension was then left undisturbed for 12 hours to allow the GO to precipitate fully.

The precipitated GO was carefully washed to remove impurities. First, the solid product was treated with 250 mL of a 1:10 Hydrochloric Acid (HCl) aqueous solution to remove residual metal ions. Subsequently, the product was washed repeatedly with distilled water until the pH of the solution reached neutrality, ensuring the removal of any remaining acid or other contaminants.

Finally, the purified GO precipitate was collected via centrifugation, which separated the solid GO from the liquid phase. The collected product was dried in an oven at 50°C for 12 hours, yielding a stable, fine powder of Graphene Oxide. This method ensures the production of high-purity GO with excellent structural and functional properties, making it suitable for advanced applications such as energy storage, water purification, and composites.

2.3. SYNTHESIS OF ZnO-GO NANOPARTICLES

ZnO-GO nanoparticles were synthesized to achieve uniform dispersion and effective integration of ZnO with Graphene Oxide. The nanoparticles were prepared in varying proportions, namely ZnO-GO 0.5%, ZnO-GO 0.75%, and ZnO-GO 1%, with the percentages corresponding to the extent of synthesized GO incorporated into the nanoparticle.

Synthesis of ZnO Dispersion: The ZnO dispersion was prepared by sonicating the required amount of ZnO in 50 mL of a homogenous ethanol-water solution (1:1 volume ratio). This process was carried out in a sonication bath for 2 hours to ensure uniform dispersion and prevent nanoparticle agglomeration. The ethanol-water mixture provided an ideal medium for stabilizing ZnO particles during the mixing process.

Synthesis of GO Suspension: Simultaneously, Graphene Oxide (GO) was dispersed in 50 mL of deionized water containing 1% Sodium Dodecyl Sulphate (SDS), a surfactant used to enhance the suspension process. SDS helps to maintain a uniform colloidal dispersion by preventing GO sheet aggregation and stabilizing the nanoparticle. The GO suspension was also sonicated for 2 hours to ensure proper exfoliation of GO and uniform dispersion.

Combining GO and ZnO: The pre-prepared GO suspension was gradually added to the ZnO dispersion in equal volumes. The combined solution was subjected to additional sonication at ambient temperature to achieve a homogenous mixture. After 30 minutes of sonication, a 1 M Sodium Hydroxide (NaOH) solution was added dropwise while stirring to adjust the pH of the mixture to 10, ensuring the stabilization of ZnO and GO in the solution.

Thermal Treatment: The resulting solution was heated in a water bath at an elevated temperature of 85°C for 5 hours to facilitate the formation of the ZnO-GO. This process improved the interaction between ZnO and GO by allowing strong interfacial bonding.

Purification and Drying: The synthesized precipitate was collected through centrifugation and thoroughly washed with deionized water three times to remove any residual impurities, including SDS and NaOH. Finally, the purified nanoparticle was dried in a vacuum oven at 50°C for 5 hours to ensure the removal of solvent traces and to obtain a stable ZnO-GO.

2.4. ANALYTICAL METHODS UTILIZED

2.4.1. X-RAY DIFFRACTION TECHNIQUE

X-ray diffraction (XRD) is a widely utilized analytical technique for characterizing the structural, crystallographic, and phase properties of materials. It is particularly significant in the study of nanomaterials, providing essential information about phase identification, crystallite size, lattice parameters, and crystallinity. The method relies on the interaction of X-rays with the periodic atomic arrangements in crystalline solids, generating diffraction patterns that serve as unique fingerprints for material characterization.

a. PRINCIPLE OF XRD

The principle of XRD is based on Bragg's Law, which establishes the relationship between the wavelength of the incident X-rays (λ), the interatomic spacing of the crystal lattice (d), and the diffraction angle (θ). This relationship is mathematically expressed as:

$$n\,\lambda = 2d \sin \theta$$

Where n is the order of diffraction. Constructive interference occurs when the incident X-rays meet this condition, resulting in distinct diffraction peaks. These peaks correspond to specific crystallographic planes in the material, providing insights into its structural and phase characteristics.

Bragg’s Law is fundamental to XRD as it enables the identification of crystallographic planes and the calculation of lattice parameters. The diffraction pattern generated by XRD provides information about the arrangement of atoms within the crystal lattice, aiding in the determination of structural properties. This principle is particularly useful for nanomaterials, where the nanoscale effects influence diffraction patterns and peak broadening.

a. X-RAY DIFFRACTOMETER

X rays are high frequency, low wave length EM waves having wavelength in the range of 0.01 to 0.7 nm. These wave length is much enough to take place Bragg’s diffraction as the interplanar distance is comparable with the wavelength of X-rays. When the target material is bombarded with the X-rays, the photons get scattered in different directions. These scattered photons will produce constructive and destructive interference according to their phase difference. i.e. in phase waves will produce a constructive interference pattern and those in out of phase will produce destructive interference. The atoms in an crystal can be treated as a periodic array of coherent scatterers. The diffracted beams from different planes of atom will produces a diffraction pattern .The plot of intensity of x-rays scattered at different angles by a sample is called an x-ray diffraction pattern. The scattered beams are again concentrated and focused by the receiver side optics. These focused beams are captured by the detector. Let θ be the angle between source and sample and 2 θ be that angle between incident beam and detector. Then intensity readings are plotted as the function of glazing angle 2θ°. The components are:

- Source of X-ray beams
- Incident beam and receiver side optics : used to concentrate or focus the incident and scattered X-rays.
- Goniometer : serves as the platform to hold the sample and used to orient the sample in correct orientation to produce diffraction.
- Sample holder : used to hold the sample
- Detector : Counts the number of scattered X-ray beams

The Scherrer equation is used to estimate crystallite size (D) in nanomaterials based on the broadening of diffraction peaks:

$$D= \frac{K\lambda}{\beta cos\theta}$$

Where D is the average crystallite size, K is a dimensionless shape factor (commonly 0.9), λ is the X-ray wavelength, β is the full width at half maximum (FWHM) of the peak in radians, and θ is the Bragg angle. This equation highlights the inverse relationship between peak broadening and crystallite size, making it indispensable for nanoscale material characterization.

2.4.2. FOURIER TRANSFORM INFRARED SPECTROSCOPY (FTIR)

Fourier Transform Infrared Spectroscopy (FTIR) is a widely used analytical technique for identifying chemical bonds and functional groups in materials. It is a powerful tool for understanding the molecular structure, chemical composition, and interactions within materials. FTIR spectroscopy measures the absorption of infrared radiation by a material, providing a unique fingerprint based on its molecular vibrations. This technique is particularly significant in the analysis of nanomaterials and composites, as it offers insights into surface chemistry, functionalization, and bonding interactions.

a. PRINCIPLE OF FTIR

FTIR operates on the principle of molecular vibrations, where infrared radiation is absorbed at specific wavelengths, causing molecular bonds to vibrate in stretching, bending, twisting, or rocking modes. These absorption wavelengths correspond to distinct energies unique to particular functional groups, enabling material identification. The technique follows Beer-Lambert's law, where absorbance (A) is proportional to the path length (l) and concentration (c) of the absorbing species:

$$A = \varepsilon l c$$

where ε is the molar absorptivity, a molecule-specific constant. The FTIR spectrum, plotted as absorbance or transmittance versus wavenumber (cm^{-1}), provides a chemical fingerprint of the material. The Fourier Transform algorithm converts raw time-domain interferograms into frequency-domain spectra, ensuring high-resolution identification of functional groups and molecular structures.

The components are:

- **Infrared Radiation Source:** Typically a Globar (Silicon Carbide) or Nernst glower, emitting a continuous spectrum across the mid-infrared (4000–400 cm^{-1}) region where most molecular vibrations occur.
- **Interferometer:** Modulates infrared light using a beam splitter, fixed mirror, and movable mirror to create an interference pattern encoding sample information.
- **Sample Holder:** Ensures proper sample exposure in solid, liquid, or gas states. Solids are analysed via ATR or KBr pellet methods, liquids using infrared-transparent cells, and gases in long-path cells for enhanced sensitivity.
- **Detector:** Converts transmitted or reflected infrared light into an electrical signal. DTGS detectors are used for general applications, while MCT detectors offer high sensitivity.

The Fourier Transform algorithm processes the interferogram into a spectrum, where peak positions, intensities, and shapes provide insights into chemical composition, bonding, and molecular interactions. Advanced software compares observed spectra with reference libraries for accurate material identification.

2.4.3. UV-VISIBLE SPECTROSCOPY

UV-visible (UV-Vis) spectroscopy is a potent analytical technique that investigates the absorption, transmission, and reflection of ultraviolet and visible light by substances. UV-Vis spectroscopy involves exposing a sample to light in the UV-Vis range (usually 190 to 900 nm) and measuring how much light is absorbed or transmitted using a spectrophotometer. This absorption or transmission spectrum provides valuable information about the electronic structure, concentration, and chemical environment of the sample's molecules. The working principle of UV-Vis spectroscopy involves passing a beam of UV or visible light through a sample, where it interacts with the sample's molecules. Some of the light is absorbed by the molecules, promoting electrons to higher energy levels, while the remaining light is transmitted through the sample. A detector monitors the intensity of transmitted light, and the absorbance spectrum is calculated by graphing the logarithm of the ratio of incident to transmitted light intensity against wavelength. UV-Vis spectroscopy relies on the Beer- Lambert law, which states that absorbance is proportional to the concentration of the absorbing species, the path length of the light through the sample, and the molar absorptivity (extinction coefficient) of the species at a given wavelength. By comparing the absorbance of a sample to a calibration curve or reference standards, the concentration of the analyte can be determined accurately. It is commonly used for quantitative analysis, determining the concentration of analytes in solution based on the Beer-Lambert law, which relates absorbance to concentration and path length.

2.4.4. PHOTOLUMINESCENCE SPECTROSCOPY

Photoluminescence (PL) Spectroscopy is an optical method of non-destructive material characterization, especially suited for semiconductors, insulators, and nanomaterials. It elucidates bandgap energy, defect levels, impurity states, and crystallinity based on the analysis of light emission following photon excitation. The technique has become vital in optoelectronics, LEDs, laser diodes, and photovoltaics as it assists in measuring material purity, structure integrity, and defect density, rendering it a powerful tool in high-performance electronic and photonic devices development.

The principle of photoluminescence is based on the absorption of photons by a material, followed by the emission of light as the material returns to its ground state. When a material is exposed to light with energy equal to or greater than its bandgap, electrons are excited from the valence band to the conduction band, leaving behind holes. These excited electrons eventually recombine with holes, emitting photons. The emitted light's energy corresponds to the material's electronic transitions and can be used to determine the bandgap and defect states. The energy of the emitted photon can be described by the relation:

$$E = h\nu = E_g - E_{\text{defects}}$$

where E_g is the bandgap energy and E_{defects} accounts for defect or impurity levels involved in the recombination process. This emission is typically categorized into near-band-edge (NBE) emission, related to excitonic recombination, and deep-level emission (DLE), associated with defects and impurities.

Photoluminescence (PL) spectroscopy comprises several main parts that excite a sample and measure its luminescent radiation. The source of excitation can be either a laser or xenon lamp, with the selection of an appropriate wavelength performed using a monochromator or optical filter. The sample is typically situated on a temperature-controlled sample holder, emits radiation when excited, and is gathered using optical lenses or fibre optics and then led into a spectrometer. A photomultiplier tube (PMT) or charge-coupled device (CCD) measures the dispersed light and transforms it into an electrical signal analysed by software to produce a PL spectrum, which displays the electronic properties of the material.

PL spectroscopy finds widespread application in semiconductors, nanotechnology, and optoelectronics for measuring bandgap energy, defect levels, and material quality. It assists in the optimization of materials such as Si, GaAs, and ZnO for LEDs, laser diodes, and solar cells, and facilitates the study of quantum confinement effects in nanostructures such as quantum dots and nanowires. It also evaluates thin film uniformity and contamination.

One of the greatest benefits of PL is that it is non-destructive and can detect even very small defects within both bulk and nanoscale materials. It does have the drawback of only working with optically active materials and needing control for its measurement wavelengths and conditions, though.

2.4.5. ANTIBACTERIAL ANALYSIS

Antibacterial testing measures the capacity of compounds to prevent or kill bacterial growth, an important aspect of creating antimicrobial agents for healthcare, food protection, and environmental use. Testing gives information about the efficacy of antibacterial materials and their action mechanisms.

Test methods include the disk diffusion assay, in which inhibition zones are a measure of antibacterial activity, the broth dilution assay, which establishes the minimum inhibitory concentration (MIC), and the agar well diffusion assay, which assesses bacterial susceptibility to the test compound. These tests quantify antibacterial efficiency and inform the creation of new antimicrobial drugs.

The well agar diffusion assay (shooting method) is an effective technique for assessing antibacterial activity of compounds such as ZnO-GO nanoparticles against bacteria like *Escherichia coli* and *Staphylococcus aureus*. Unlike the disk diffusion method, this approach involves inoculating Mueller-Hinton agar plates uniformly with a standardized bacterial suspension adjusted to a 0.5 McFarland standard. Small wells (5–8 mm in diameter) are then created within the agar using a sterile cork borer or micropipette tip, followed by precise dispensing (“shooting”) of 20–100 μL of nanoparticle suspension into each well, ensuring no air bubbles or overflow. Plates are incubated at 37°C for 18–24 hours, after which clear zones of inhibition around the wells indicate antibacterial activity. These inhibition zones are measured accurately to compare efficacy across different samples or concentrations. The method accommodates larger sample volumes than disk diffusion, offering increased sensitivity particularly for substances with limited diffusion, although it requires careful control of well dimensions, volume consistency, and bacterial inoculation to ensure reliable results.

Antibacterial materials find extensive usage in healthcare, food preservation, and water treatment. Antimicrobial coatings on medical devices prevent infections in the field of medicine, while in food, antibacterial packaging reduces shelf life by limiting microbial contamination. In water treatment, antibacterial agents kill harmful pathogens, providing safe drinking water. As antibiotic resistance continues to rise, antibacterial analysis remains critical to drive effective and sustainable antimicrobial solutions.

CHAPTER 3

3. RESULTS AND DISCUSSIONS

3.1. X-RAY DIFFRACTION STUDIES

a. ZnO

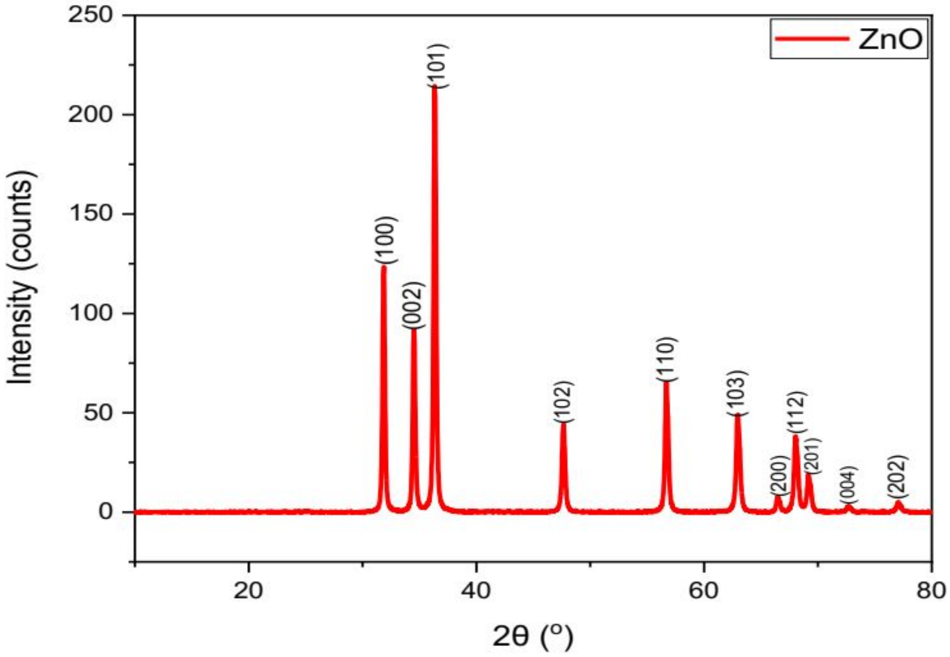


Fig 3.1 XRD patterns of ZnO sample.

Figure 3.1 shows XRD plot of ZnO sample observed at 40kV and 35 mA(Cukα: λ=1.54 Å) which was plotted and analysed using Origin software. The major peaks are observed at: 31.86°, 34.52°, 36.36°, 47.66°, 56.72°, 62.99°, 66.51°, 68.08°, and 69.21°.

The (100), (002), (101), (102), (110), (103), (200), (112), (201), (004), and (202) lattice planes were observed at 31.86°, 34.52°, 36.36°, 47.66°, 56.72°, 62.99°, 66.51°, 68.08°, and 69.21° respectively. This confirmed that the obtained ZnO has wurtzite hexagonal structure. The average size (D) of the samples can be calculated using Debye-Scherrer formula as shown in equation,

$$D = \frac{K\,\lambda}{\beta \cos\theta}$$

Here, K represents the shape factor, with a specific value of 0.9678. The symbol λ corresponds to the wavelength of Cu-Kα radiation (1.54 Å), θ denotes Bragg's angle measured in degrees, and β signifies the Full Width at Half Maximum (FWHM) of the diffraction peak. This formula serves as a means to estimate the average size of crystalline samples based on X-ray diffraction data, providing valuable insights into the structural characteristics of the material under investigation.

The 2θ value of major peak, average crystallite size (D), FWHM values of the sample are analysed in table 3.1.

Peak position (2 θ)	FWHM	2 θ(radian)	θ (radian)	Crystallite size D(nm)	**Average Crystallite size, D (nm)**
31.86	0.26	0.55	0.27	30.69	25.44
34.52	0.29	0.60	0.30	28.58	
36.35	0.29	0.63	0.31	28.79	
47.65	0.34	0.83	0.41	25.44	
56.71	0.36	0.98	0.49	24.89	
62.98	0.42	1.09	0.54	22.11	
66.51	0.44	1.16	0.58	21.14	
68.08	0.43	1.18	0.59	21.83	
69.21	0.46	1.20	0.60	20.73	
77.09	0.39	1.34	0.67	25.64	
81.52	0.34	1.42	0.71	29.99	

Table 3.1 Crystallite Size Calculation of ZnO

The crystallite size was measured as 25 nm. This measurement indicates that the synthesized nanoparticles exhibit nanoscale crystallinity. The observed crystallite size, derived from X-ray diffraction (XRD) peak broadening, suggests that the synthesized nanoparticles are finely crystalline and uniform, consistent with effective control of particle growth during synthesis. The obtained peaks were compared with JCPDS file of ZnO(00-036-1451).

b. GO

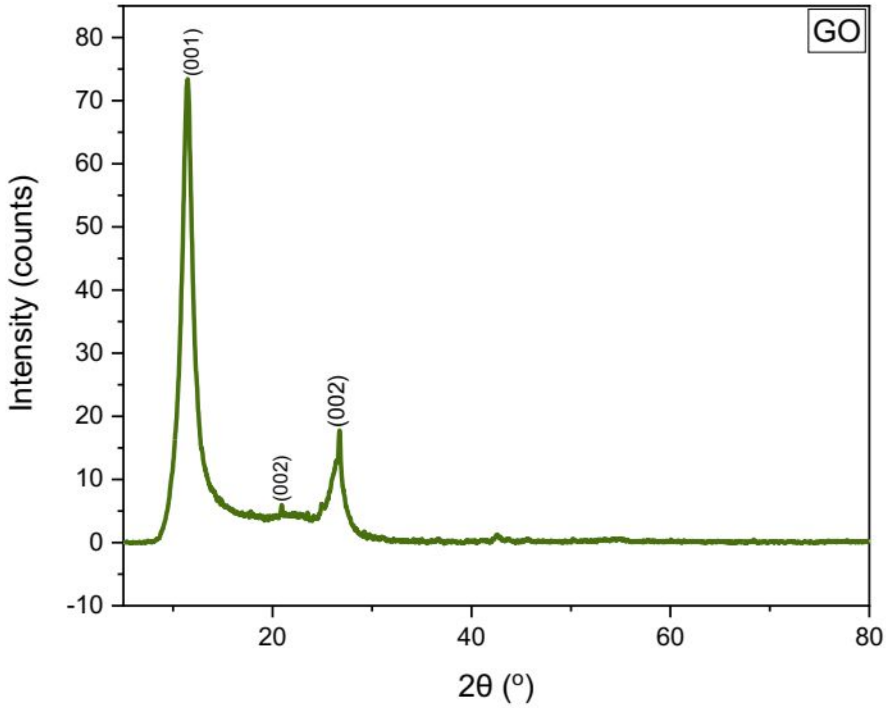


Fig 3.2 XRD patterns of GO sample.

XRD analysis revealed two broad peaks at 11.42° and 26.52°, and a smaller peak at 20.7°. The peak at 11.42° corresponds to the (001) plane of GO, while the peaks at 26.52° and 20.7° are associated with the (002) plane of GO. The peak (002) observed at 20.7° was broader and had lower intensity than the natural graphite and represents the Graphene with reduced layers. Crystallite size calculations were performed using the Debye–Scherrer formula based on these observed peaks.

Peak position (2 θ)	FWHM	2 θ(radian)	θ (radian)	Crystallite size D (nm)	**Average crystallite size, D (nm)**
11.41	1.60	0.19	0.09	4.96	5.10
26.51	1.55	0.46	0.23	5.24	

Table 3.2 Crystallite Size Calculation of GO

The crystallite size was measured as 5.1 nm, indicating nanoscale crystallinity and uniformity of synthesized nanoparticles, confirmed by X-ray diffraction (XRD) analysis. The identification and structural confirmation of Graphene Oxide (GO) in the nanoparticle were supported by characteristic peaks observed in the diffraction pattern, aligning closely with standard reference data. The obtained peaks were compared with JCPDS file of GO (00-065-1528).

c. ZnO - GO

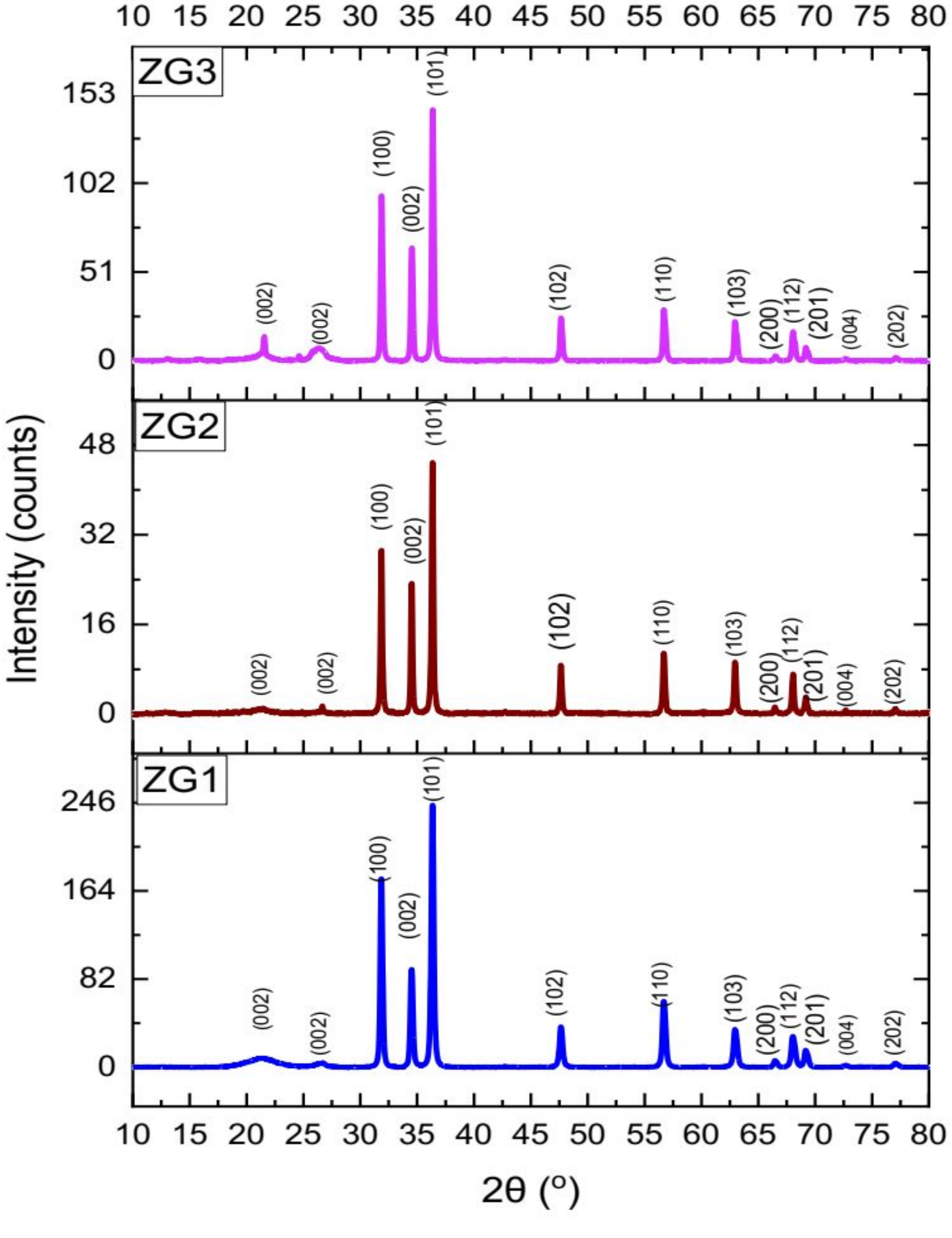


Fig 3.3 XRD patterns of ZG1, ZG2 and ZG3 sample.

ZnO-GO nanoparticles were synthesized in three different compositions based on weight percentage (wt%): ZG1 at 0.5 wt%, ZG2 at 0.75 wt%, and ZG3 at 1 wt%. The figure shows XRD pattern that reveals characteristic peaks corresponding to both ZnO and GO, confirming the successful integration of ZnO with Graphene Oxide sheets. Additionally, the presence of broad peaks at 21.34° and 26.41° indicates the structural incorporation of GO within the composite.

	Peak position (2 θ)degree)	FWHM	2 θ) (radian)	θ(radian)	**Crystallite size, D(nm)**
ZG1	47.74	2.45	0.83	0.41	21.46
ZG2	47.81	2.27	0.83	0.41	37.71
ZG3	47.57	5.05	0.83	0.41	22.18

Fig 3.3 Crystallite Size Calculation of ZG1, ZG2 and ZG3

Averages of Peak positions, FWHM, theta values and crystallite size of ZG1, ZG2, ZG3 are depicted in the above table. The crystallite sizes obtained for the prepared ZnO-GO nanoparticles were measured as 21.46nm for ZG1, 37.71nm for ZG2 and 22.19 nm for ZG3, indicating variation with different GO concentrations.

3.2. FOURIER TRANSFORM INFRARED SPECTROSCOPY (FTIR)

FTIR analysis can be used to confirm the formation of a composite material by detecting changes in the infrared absorption spectra of the individual components after they have been combined. A Fourier Transform Infra-Red Spectrophotometer (IRAffinity-1) was used to get the FTIR spectrum. Figure 3.4 depicts the FTIR spectroscopic plot created with the origin software.

The absorption spectrum reveals distinct bands corresponding to specific functional groups in the material. The ZnO exhibit absorption peak at 874 cm^{-1} is attributed to ZnO stretching. Additionally, the band at 1325 cm^{-1} corresponds to epoxide group, while C-O group vibrations manifest at 2339 cm^{-1}.

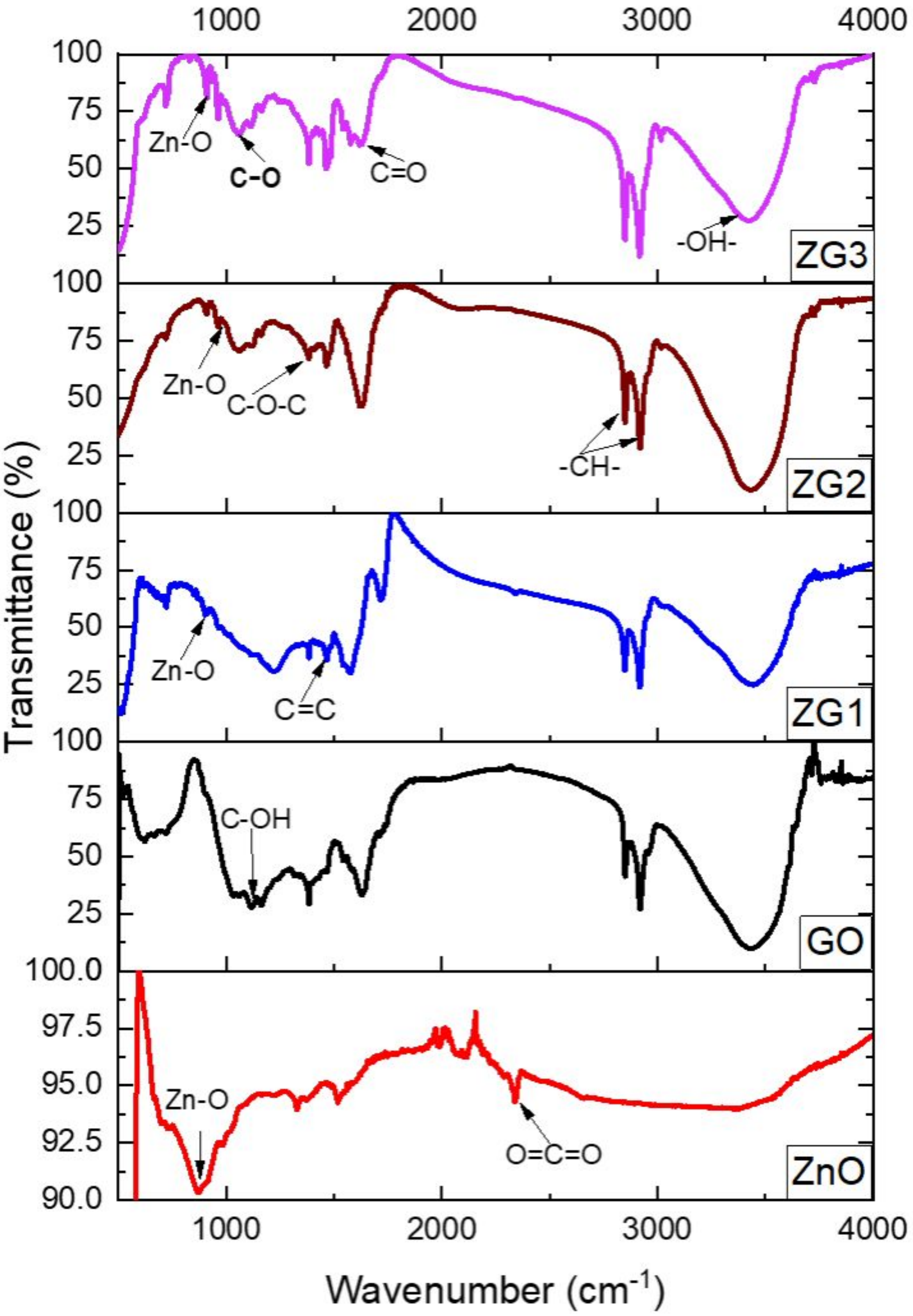


Fig 3.4: FTIR spectra for ZnO, GO, ZG1, ZG2, ZG3 samples.

Graphene Oxide (GO) exhibited characteristic peaks corresponding to various functional groups. Peaks were observed at 1127 cm^{-1} representing the C–OH stretching, 1393 cm^{-1} for the C–O–C stretching vibration, and 1634 cm^{-1} corresponding to the C=O stretching vibration. Additionally, peaks at 2851 cm^{-1} and 2915 cm^{-1} indicate the presence of C–H (alkane) and C=H (alkene) stretching vibrations, respectively. A broad peak at 3447 cm^{-1} confirms the presence of hydroxyl (–OH) groups. These characteristic peaks confirm the successful formation and oxidation of GO.

The FTIR spectrum of ZnO-GO nanoparticle reveals bands representing both ZnO and GO, and the collective information indicating the formation of ZnO-GO nanoparticle and the interaction between ZnO and GO.

3.3. UV ABSORPTION SPECTROSCOPY

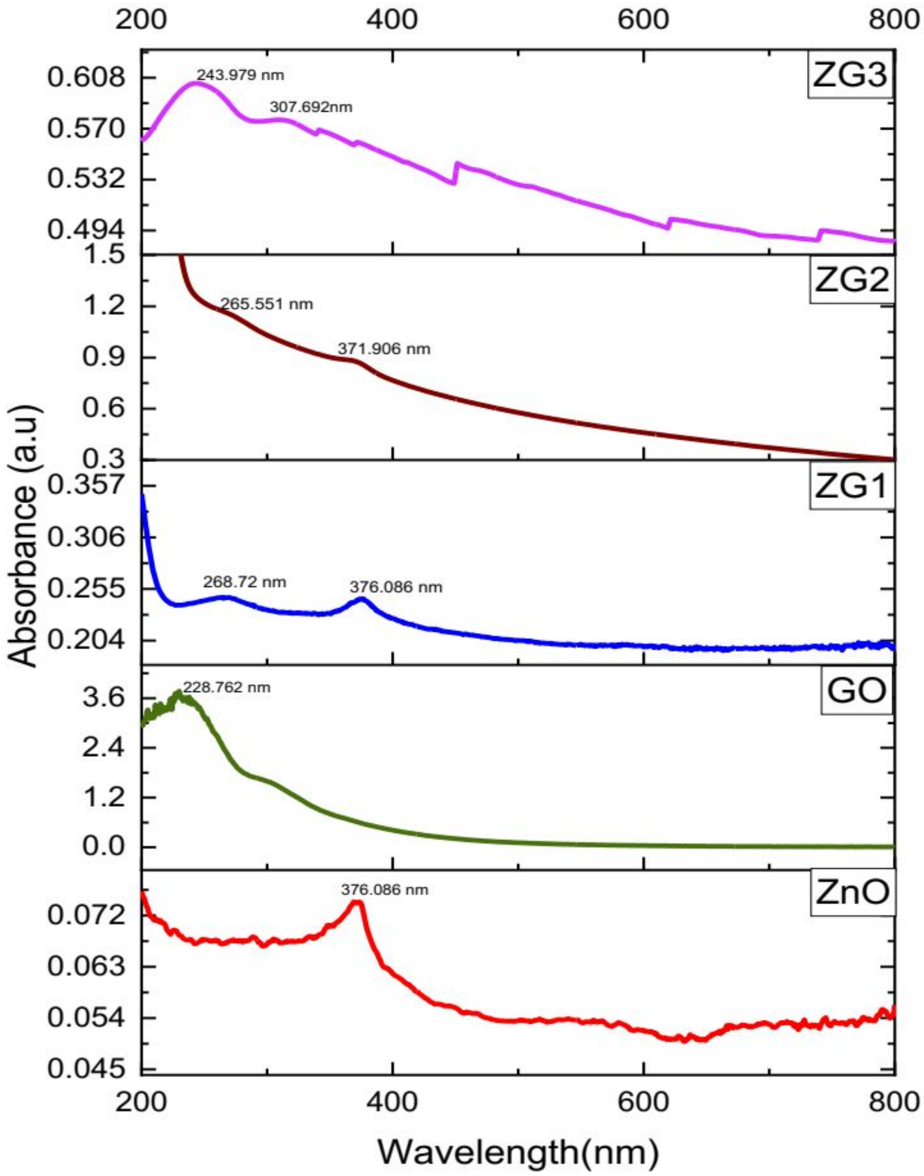


Fig 3.5: UV absorption spectra for ZnO, GO, ZG1, ZG2, ZG3 samples.

The absorption spectra of samples are obtained using the UV Visible Spectrophotometer – JASCO (V-670 PC) and are depicted in Figure 3.4. It measures the absorption of light in the UV (200–400 nm) and visible (400–700 nm) regions, providing insights into band gap energy, optical transitions, and material purity. In this study, UV-Vis spectroscopy was utilized to analyse ZnO-GO nanoparticles by evaluating their optical characteristics. Specifically, it was employed to determine the optical band gap through Tauc's plot analysis, investigate the effects of Graphene Oxide (GO) incorporation on the optical properties of ZnO, and assess changes due to compositional variations. Band gap energies were calculated from the absorption edge, yielding critical insights into the nanoparticles suitability for potential optoelectronic applications.

a. ZnO

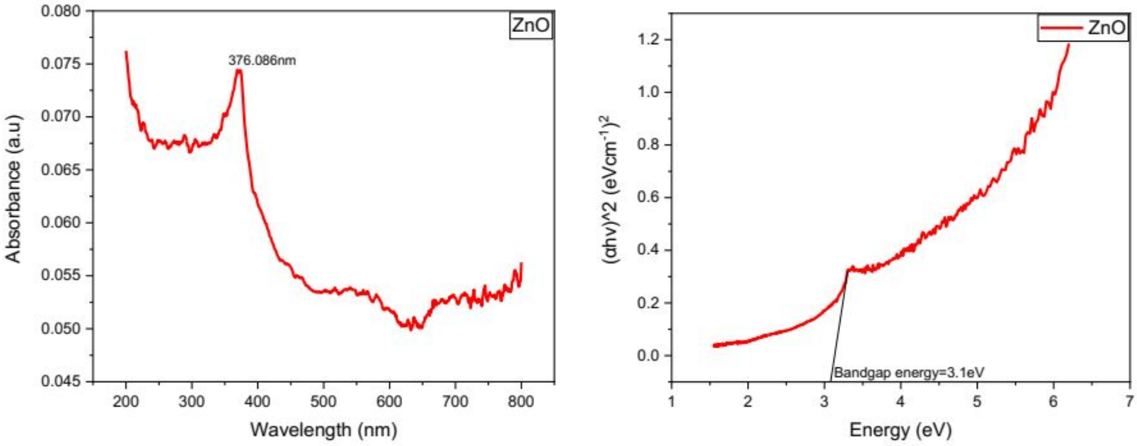


Fig 3.6: (i) UV absorption spectra, (ii) Tauc plot of ZnO.

A distinct absorption peak was observed at 376 nm, indicating the excitonic absorption characteristic of ZnO. This clear and sharp peak confirms the presence of ZnO, signifying good crystallinity and structural quality in the synthesized material.

The determination of the sample's bandgap energy relies on the Tauc plot method. This method involves analysing the absorption spectrum of a material by measuring the absorption coefficient (α) at various photon energies using UV-visible spectroscopy. The subsequent step includes constructing a Tauc plot, where $(\alpha h v)1/n$ (with n being 1/2 for a direct bandgap) is graphed against photon energy (hν). The linear segment of this plot is then identified and extrapolated to the x-axis (hν). The point at which the extrapolated line intersects the x-axis represents the bandgap energy (Eg) of the material. This determination holds significance in semiconductor physics, materials science, and applications related to photovoltaics. The Tauc plot methodology is grounded in the Tauc equation, establishing a correlation between the absorption coefficient and the energy of incident photons near the absorption edge. The Tauc plot thus obtained is shown in figure 3.5 (ii). The band gap energy of sample ZnO is found out to be 3.1eV.

b. GO

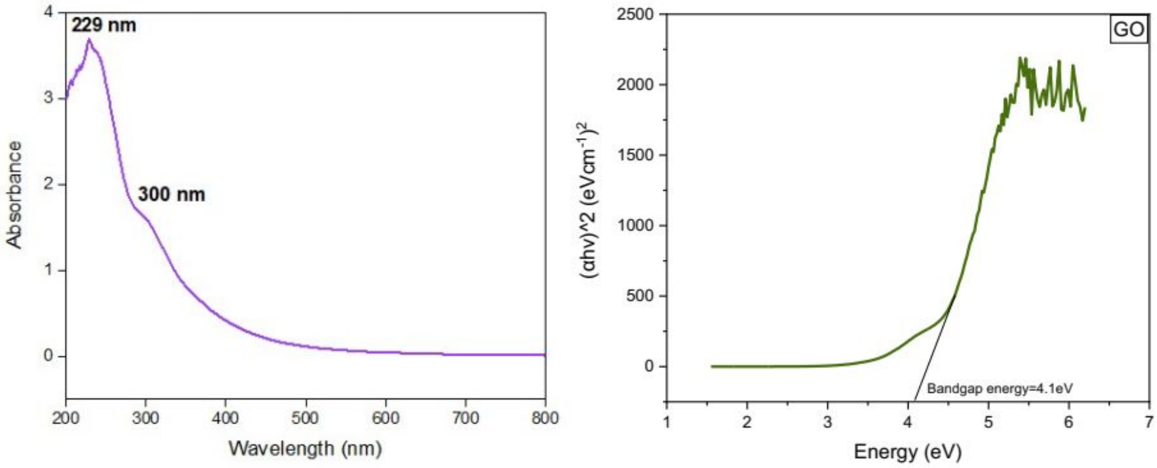


Fig 3.7: (i) UV absorption spectra, (ii) Tauc plot of GO.

Graphene Oxide (GO) exhibited a prominent absorption peak at 228 nm, corresponding to the $\pi \rightarrow \pi^*$ electronic transition of the aromatic C=C bond. Additionally, a shoulder peak observed is attributed to the $n \rightarrow \pi^*$ transition. These characteristic absorption features indicate the presence of sp^2-hybridized carbon atoms, confirming the successful formation and structural integrity of GO. The band gap energy of sample GO is found out to be 4.1 eVfrom the Tauc plot in figure 3.6(ii).

c. ZnO – GO

The UV-Vis spectrum of the ZnO-GO nanoparticle exhibited peaks corresponding closely to those observed separately in ZnO and GO, confirming the successful integration of ZnO with Graphene Oxide. ZG1, ZG2 and ZG3 exhibited prominent peaks at 268.72nm, 265.55nm and 243.97nm respectively depicting the $\pi \rightarrow \pi^*$ electronic transition of the aromatic C=C bond indicating graphite contribution. Meanwhile the peaks at 367.08nm, 371.906nm and 307.69nm corresponds to excitonic absorption characteristic of ZnO.

Using Tauc's plot, the optical band gap values calculated for the composites were found to vary based on GO concentration, with measured values of 0.5 wt% (ZG1), 0.75 wt% (ZG2), and 1 wt% (ZG3). The bandgap energies calculated from the Tauc plots are as follows: ZG1 = 5 eV, ZG2 = 4.8 eV, and ZG3 = 3.1 eV. This analysis highlights the trend that increasing GO content significantly affects the optical properties, particularly reducing the band gap energy, thereby enhancing the nanoparticle's potential for optoelectronic applications.

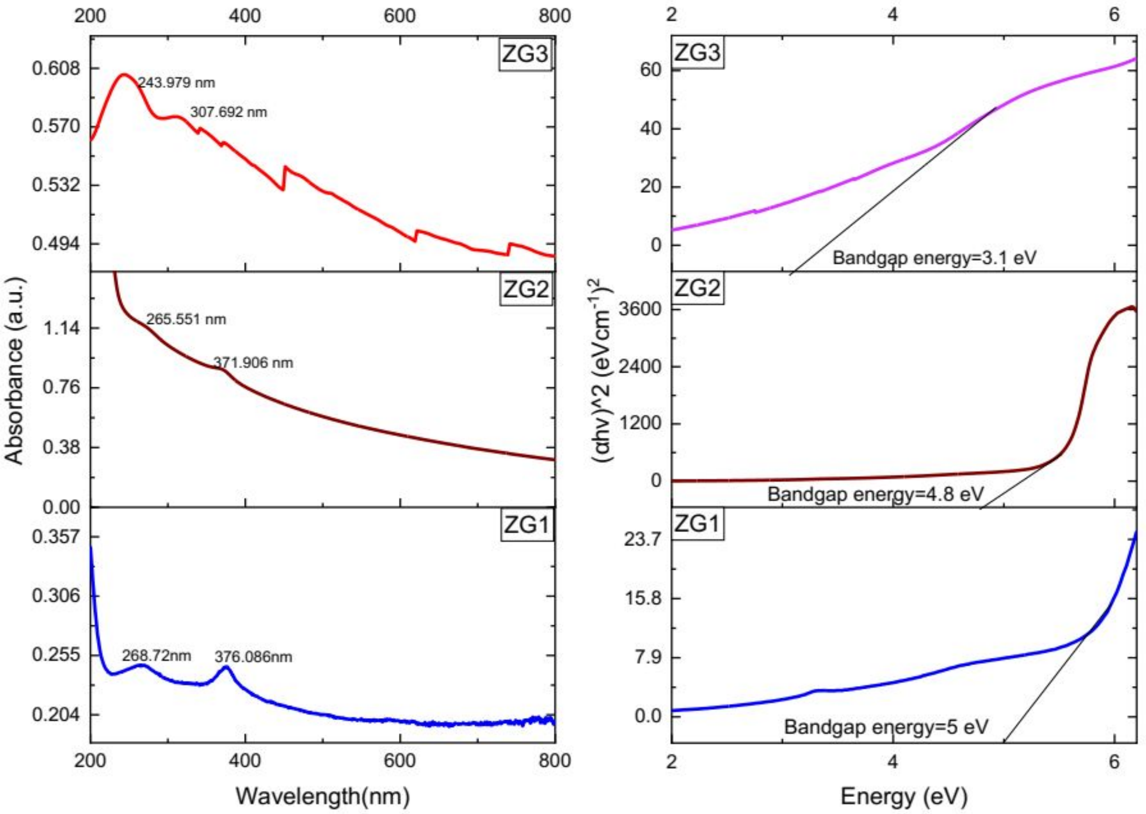


Fig 3.8: (i) UV absorption spectra, (ii) Tauc plots of ZG1, ZG2, ZG3.

3.4. PHOTOLUMINESCENCE PROPERTIES

Photoluminescence (PL) spectroscopy is an important technique used to study the optical properties, electronic transitions, and defect states of semiconductor materials. In this study, PL spectroscopy was utilized to analyse the emission behaviour of ZnO, GO and ZnO-GO nanoparticles, identify defect states such as Oxygen vacancies, Zinc interstitials, and surface defects, and investigate the influence of GO incorporation on ZnO's luminescence intensity and recombination dynamics. The obtained PL spectra revealed key emission peaks, allowing for a clear understanding of GO's role in modifying the optical properties of ZnO, which is essential for applications in optoelectronics, sensors, and photocatalysis. Furthermore, PL studies were conducted at different excitation wavelengths—300 nm, 325 nm, and 350 nm—and these experiments resulted in similar emission profiles. Among these, the PL profile excited at 300 nm provided a detailed basis for further discussion.

a. ZnO

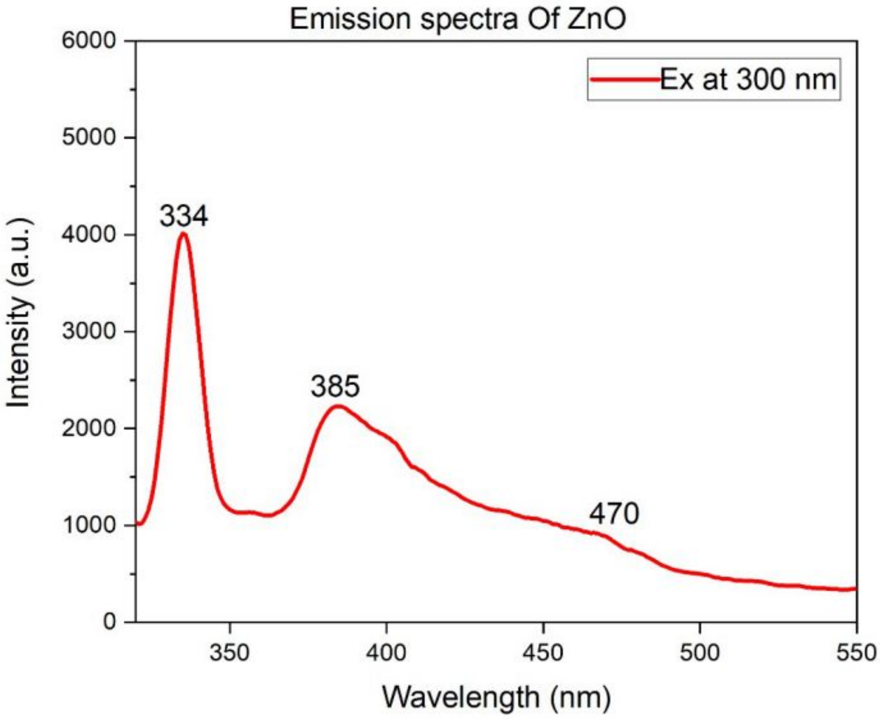


Fig 3.9: PL emission spectra for ZnO sample.

The emission peak at 334 nm corresponds to near-band-edge (NBE) emission, indicating excitonic recombination, while the peak observed at 385 nm is attributed specifically to the recombination of excitons. Additionally, the visible emission peak at 470 nm arises from various intrinsic defects within the material, including Oxygen vacancies, Zinc vacancies, Oxygen interstitials, Zinc interstitials, and Oxygen antisites.

b. GO

The emission peak at 335 nm in the UV region arises from the recombination of electron-hole pairs within the small sp^2 domains of GO. The peak observed at 670 nm in the red region is attributed to emissions from Oxygen-containing functional groups, specifically carbonyl (C=O) and carboxyl (COOH) groups located at the edges of GO, indicating a high density of Oxygen-rich functionalities. These particular peak positions (335 nm and 670 nm) suggest that the GO preparation method employed in this study successfully produced a material characterized by both isolated aromatic regions and substantial edge functionalization with Oxygen-containing groups.

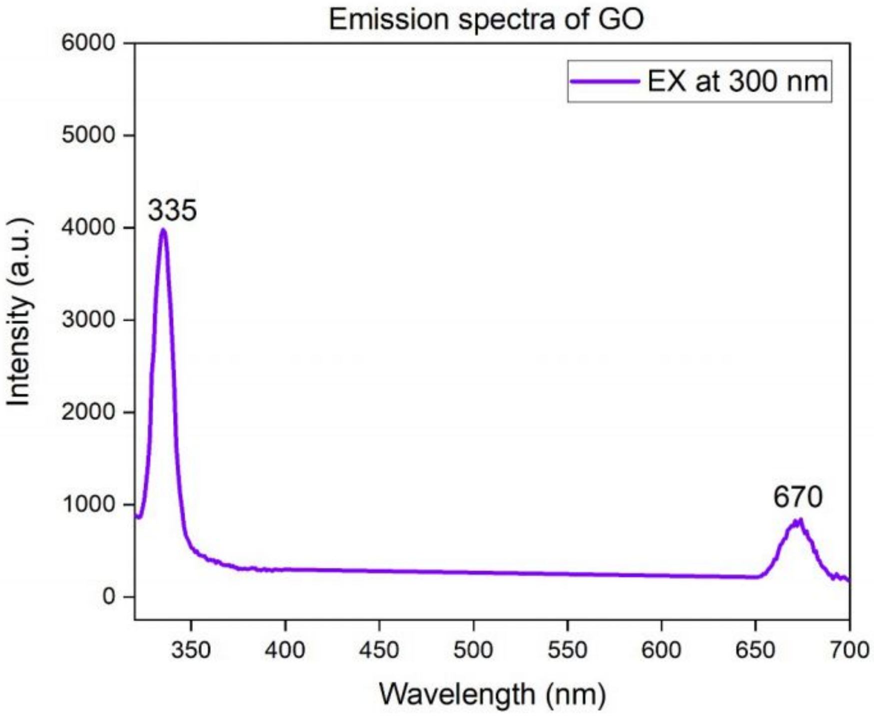


Fig 3.10: PL emission spectra for GO sample.

c. ZnO – GO

The emission peak at 336 nm corresponds to the near-band-edge (NBE) emission of ZnO, signifying excitonic recombination. The peak observed at 380 nm is attributed to electron-hole recombination processes. Additionally, the emission peak at 470 nm, observed in samples ZG2 and ZG3, likely arises from deep-level defect states, specifically Oxygen vacancies or Zinc interstitials within the material.

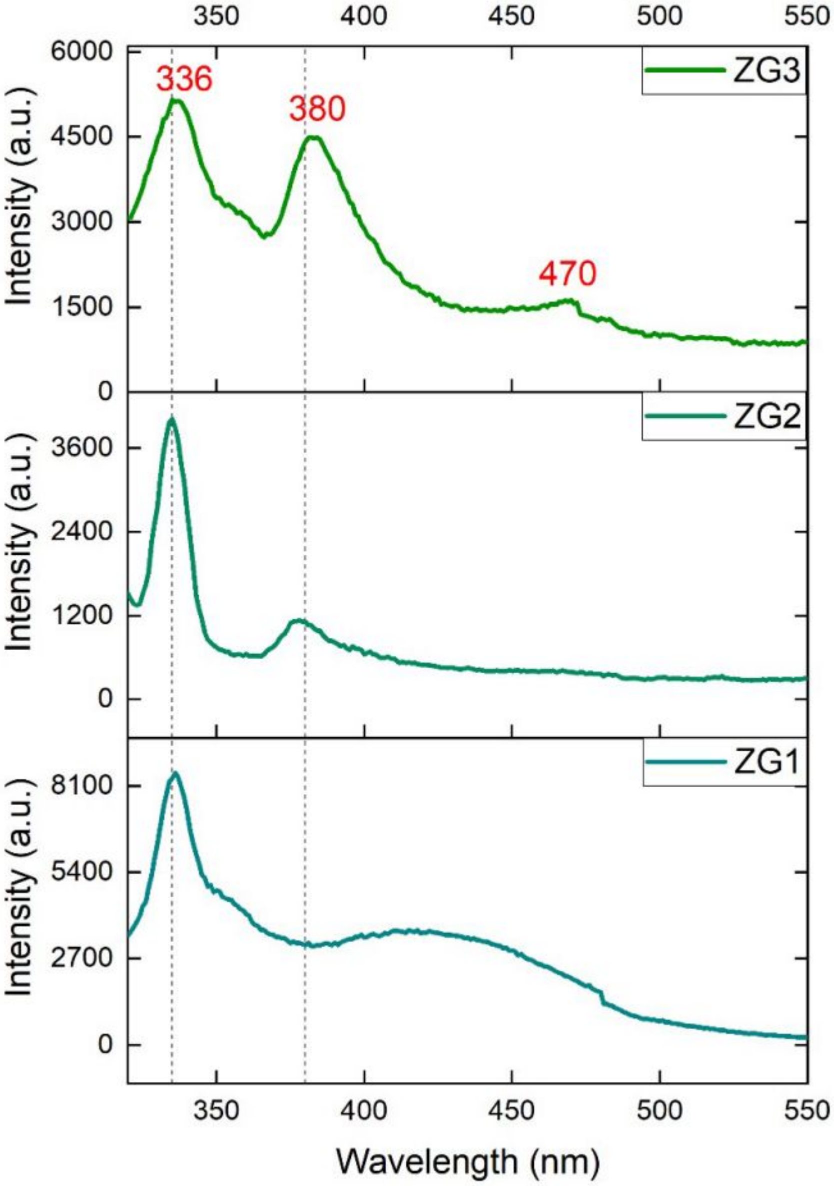


Fig 3.11: PL emission spectra for ZG1, ZG2, ZG3 samples excited at 300nm.

3.5. ANTIBACTERIAL ACTIVITY

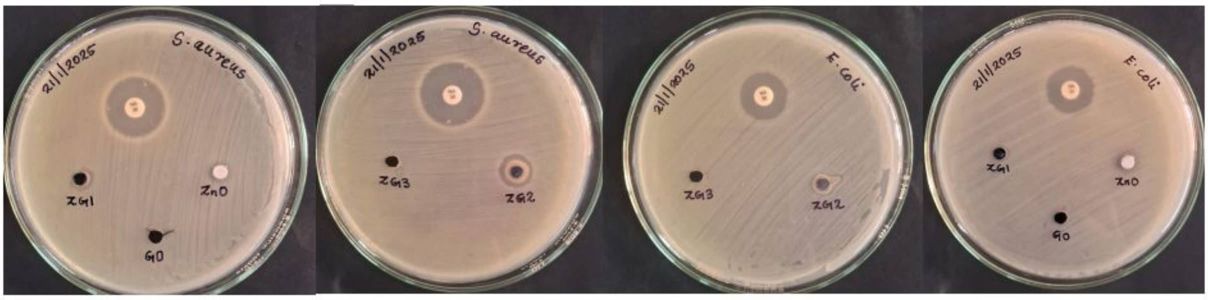
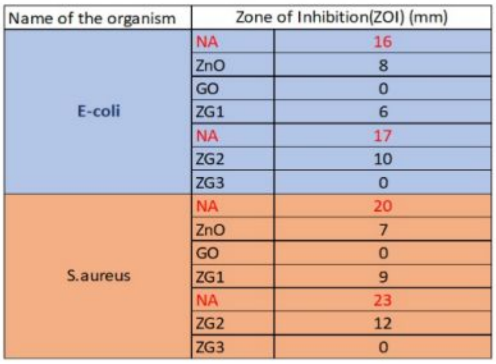


Fig 3.12 Antibacterial activity of ZnO, GO, ZG1, ZG2 and ZG3 under E-coli and S.aureus in Trial -1

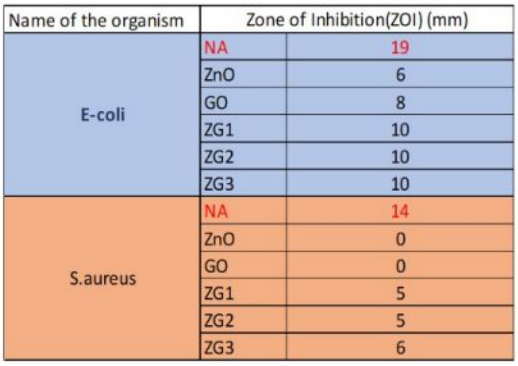
Against *E. coli*, the samples ZG1, ZG2, and ZG3 displayed larger zones of inhibition compared to pure ZnO and GO, indicating enhanced antibacterial properties. However, their antibacterial activity remains lower than that of the reference antibiotic. Against *S. aureus*, pure ZnO and GO showed no significant antibacterial activity, whereas ZG1, ZG2, and ZG3 exhibited measurable zones of inhibition, confirming their antibacterial efficacy to some extent. Nonetheless, the zones of inhibition for these nanoparticles were still smaller than those produced by the reference antibiotic.

Trial - 1



Name of the organism	Zone of Inhibition(ZOI) (mm)	
E-coli	NA	16
	ZnO	8
	GO	0
	ZG1	6
	NA	17
	ZG2	10
	ZG3	0
S.aureus	NA	20
	ZnO	7
	GO	0
	ZG1	9
	NA	23
	ZG2	12
	ZG3	0

Trial - 2



Name of the organism	Zone of Inhibition(ZOI) (mm)	
E-coli	NA	19
	ZnO	6
	GO	8
	ZG1	10
	ZG2	10
	ZG3	10
S.aureus	NA	14
	ZnO	0
	GO	0
	ZG1	5
	ZG2	5
	ZG3	6

Table 3.4 Inhibition zones under E-coli and S.aureus of ZnO, GO, ZG1, ZG2 and ZG3 (i) Trial - 1 (ii) Trial - 2

The synergy between ZnO and GO in the nanoparticles enhances their antibacterial effect, likely due to improved reactive Oxygen species (ROS) generation or better dispersion of ZnO particles facilitated by GO. Gram-negative bacteria (*E. coli*) appear to be more susceptible to the nanoparticles, possibly because of their thinner outer membrane structure, which makes them more vulnerable to ROS-mediated damage. In contrast, Gram-positive bacteria (*S. aureus*) exhibit lower susceptibility, potentially requiring higher concentrations of the nanoparticle or alternative antibacterial mechanisms to achieve more effective inhibition.

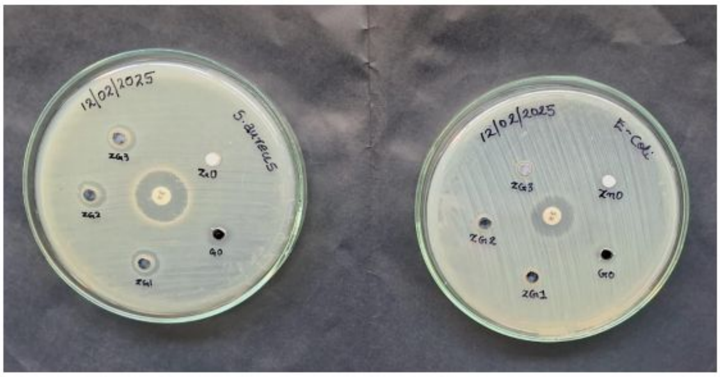


Fig 3.13 Antibacterial activity of ZnO, GO, ZG1, ZG2 and ZG3 under E-coli and S.aureus in Trial -2

Antibacterial studies demonstrated improved antibacterial activity of ZnO-GO nanoparticles compared to pure ZnO, suggesting synergistic effects between ZnO and GO but does not showed activity more than the reference antibiotic.

CONCLUSION

In this study, ZnO, GO and ZnO-GO nanoparticles were synthesized, and they were thoroughly characterized to determine their properties with respect to structure, optical aspects, and antibacterial activity. X-ray diffraction analysis confirmed the crystalline structure of ZnO and proved incorporation of Graphene Oxide (GO) into ZnO matrix without affecting the original crystal structure. Moreover, the calculated crystallite sizes showed a clear decreasing trend with the increase of GO indicating the efficiency of GO in restricting the grain growth of ZnO. Successful synthesis has also been confirmed through Fourier-transform infrared (FTIR) spectroscopy since it has characteristic vibrational modes of ZnO and distinct absorption bands linked with the functional groups that are available in GO. These results indicated successful interaction and arrangement of ZnO and GO in the nanoparticles.

Optical studies employing UV-Vis spectroscopy indicated a slight but consistent decrease in the bandgap energy of the nanoparticles as the GO concentration increased. Since the bandgap decreased with an increase in GO, it was most likely indicative of increased charge transfer and better dispersion due to the visualization of GO into the composites, which improved the optical absorption properties. Photoluminescence (PL) spectroscopy also provided valuable information regarding the optical behaviour of synthesized materials. The emission peaks were recorded at 336nm, which corresponded to near-band-edge (NBE) emission observed in all samples and was attributed to excitonic recombination. The presence of impurity-associated defect emissions at 380nm was recorded exclusively in ZG2 (0.75 wt%) and ZG3 (1 wt%) samples. Additionally, broad defect-related emissions ranging from 400–500 nm, including a weak peak at 470 nm in ZG3, suggested increased defect states with higher GO content.

Antibacterial studies demonstrated that ZnO-GO nanoparticles exhibited improved antibacterial activity compared to pure ZnO, highlighting synergistic interactions between ZnO and GO. However, the antibacterial effectiveness of the nanoparticles remained lower than that of the reference antibiotic.

FUTURE SCOPE

The properties manifested by Zinc Oxide and Graphene Oxide as different entities have great potential for applications. Thus, studying the combined product, ZnO-GO is of great significance.

We have already characterized our particles using characterization techniques like UV-Visible spectrum, X-Ray Diffraction spectrum(XRD), Fourier Transform of Infra-Red(FTIR) spectrum. Then their optical properties were studied using Photoluminescence (PL) spectra of emission wavelength range below 550 nm. This was done at three different excitation wavelengths of 300nm, 325 nm and 350 nm. It showed similar peaks in spectra in the ultraviolet(UV) and visible region. A deeper study could be done for the full range PL spectra. Anti-bacterial properties against *E-coli* and *S.aureus* bacterial cultures were also studied. It showed enhanced anti-bacterial activity in ZnO-GO nanoparticles than in ZnO and GO shown separately. An advanced study could be conducted on the results obtained to understand the optimum conditions for better actions of the three samples against the bacteria. These studies helped us to understand properties of both the nanoparticle and its synergistic effects.

In the future, the observations from UV-Visual spectrum and PL spectra could help studying photocatalytic properties of the nanoparticles in ultraviolet radiation. The similarity in properties of Zin Oxide and its cheaper cost is a great attraction to replace in-use photocatalysts. Invaluable aid of the ZnO-GO nanoparticles in water treatment applications could be studied for removal of chosen heavy metals. The study is expected to be conducted for different physical and chemical variables. Thus, the study could be taken to the next level of publishing in a journal, with comprehensive research and thorough analysis of the results obtained.

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