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FTIR and UV-VIS Characterization of ZnO Produced using Neem (*Azadirachta Indica*) Leaves Extracts

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Abstract: The growing demand for sustainable nanomaterials has intensified interest in green synthesis methods that utilize plant extracts as reducing and stabilizing agents. This research focuses on the green synthesis and characterization of zinc oxide (ZnO) nanoparticles using Neem (Azadirachta indica) leaves extract by employing simulation technique. Ultraviolet–Visible (UV–VIS) spectroscopy, Fourier Transform Infrared (FTIR) Spectroscopy and Hall-effect electrical transport properties in the other way were used to determine optical properties, functional groups with structural features and electrical transport properties respectively of the produced ZnO using simulation technique. UV–VIS spectra revealed a strong absorption peak around 360–380 nm, confirming the presence of ZnO nanoparticles and indicating a blue-shift associated with nanoscale dimensions. FTIR spectra displayed characteristic Zn–O vibrational bands between 430–500 cm^{-1}, along with phytochemical signatures responsible for reduction and capping. Hall measurements indicate n-type conductivity with carrier concentrations in the 10^{17}–10^{19} cm^{-3} range and mobilities of 8–32 $cm^2V^{-1}s^{-1}$. The findings confirm that Neem extract is an efficient biogenic agent for synthesizing ZnO nanoparticles with desirable optical and functional characteristics. The study also demonstrates that Neem-extract-mediated ZnO shows optical and electrical properties compatible with photovoltaic window layers and UV-sensing applications, while offering an eco-friendly synthesis route. The ecological and material advantages of plant-based nanoparticle synthesis were highlighted and baseline data for applications in environmental remediation, photocatalysis, and biomedical fields were provided.

Keywords: ZnO nanoparticles, Neem extract, green synthesis, FTIR, UV–VIS, Hall Effect.

I. INTRODUCTION

The prospects for using nano-materials in number of applications is being widely researched today across multiple domains such as cosmetics, optical components, pharmaceutical drug manufacture, polymer science, mechanical engineering, and toxicology to mention but few (Iravani, 2011). Energy is central to sustainable development and poverty reduction efforts in every society as it affects all aspects of development being social, economic, and environmental-including livelihoods, access to water, agricultural productivity, health, population levels, education, and gender related issues (Aiswarya *et al.*, 2023). With the ever increasing demand for energy, the search for alternative energy sources has increased. The worldwide use of fossil fuels has led to the critical situation of global warming, significantly affecting our health, environment and climate (Khalil *et al.*, 2014). Extensive emphasis have been put on the implementation of renewable energy sources and solar energy is by far the most abundant form of renewable energy (Ozgur, 2005).

Nanostructured Zinc Oxide (ZnO) materials have received broad attention due to their distinguished performance in electronics, optics and photonics, optoelectronics, sensors, transducers and biomedical sciences. From the 1960s, synthesis of ZnO thin films has been an active field because of their applications as sensors, transducers and catalysts (Abdulrahman *et al*., 2024). ZnO is therefore a key technological material. The lack of a centre of symmetry in its wurtzite structure combined with large electromechanical coupling results in strong piezoelectric and pyroelectric properties and the consequent use of ZnO in mechanical actuators and piezoelectric sensors is another considerable factor for intensifying research on ZnO. In addition, ZnO is a wide band-gap compound semiconductor that is suitable for short wavelength optoelectronic applications (Look, 2001). The high excited binding energy (60meV) in ZnO crystal can ensure efficient excitonic emission at room temperature. ZnO is transparent to visible light and can be made highly conductive by doping (Pearton, 2005).

Nanotechnology has emerged as a transformative field with applications spanning from medicine, environmental remediation, catalysis, agriculture, and electronics (Ramesh, 2016). Among various metal oxide nanoparticles, zinc oxide (ZnO) stands out due to its wide bandgap (3.37 eV), high exciton binding energy, optical clarity, and antibacterial

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properties. Conventionally, ZnO nanoparticles are synthesized using chemical methods that rely on hazardous reagents, generating toxic by-products that have negative consequences to ecosystems and human health (Kumar & Yadav, 2022). Green synthesis addresses these consequences by employing plant extracts rich in bioactive compounds to reduce and stabilize metal ions (Adam *et al*., 2021). Neem (Azadirachta indica) contains flavonoids, terpenoids, alkaloids, tannins, and phenolics, making it an excellent candidate for nanoparticle biosynthesis (Sundrarajan & Gowri, 2011). This study expands on the characterization of ZnO nanoparticles synthesized using Neem leaves extract.

Nowadays, the scientific community has increasingly turned to green synthesis, which integrates biological materials, including bacteria, fungi, and plants to produce nanoparticles in an eco-friendly manner (Singh, 2021). Plants offer major advantages due to their abundance, safety, simplicity and less cost of extraction, and diverse phytochemicals, which naturally act as reducing, stabilizing, and capping agents (Ahsan *et al. 2023)*.

Neem (Azadirachta indica) is widely recognized across tropical regions for its medicinal and antimicrobial properties. Neem leaves contain bioactive compounds such as flavonoids, alkaloids, terpenoids, tannins, and phenolic compounds. These constituents facilitate the reduction of zinc salts and stabilize the resulting nanoparticles (Ali *et al.,* 2024).

Characterization remains crucial in understanding nanoparticle properties. FTIR spectroscopy determines functional groups responsible for reduction and capping, while UV–VIS spectroscopy provides information on optical features and band gap energy. Hall effect on the other hand reveals the electrical transport properties. Together, these techniques verify the synthesis route and quality of ZnO nanoparticles for human needs applications (Khaing *et al*., 2018).

While previous studies have explored Neem-mediated synthesis of ZnO nanoparticles, there is limited systematic investigation of FTIR, UV–VIS, Hall-effect electrical transport properties which are essential for evaluating the suitability of ZnO for applications in photovoltaics, sensors, and transparent electronics. This study investigates the synthesis of ZnO nanoparticles using Neem leaf extracts, followed by FTIR, UV–VIS and Hall Effect characterization. The work contributes to environmentally friendly nanoparticles production and enhances understanding of biogenic ZnO's functional attributes.

II. MATERIALS AND METHODS

2.1 Materials

- Fresh Neem (Azadirachta indica) leaves
- Zinc nitrate hexahydrate [$Zn(NO)_2 \cdot 6H_2O$]
- Distilled water
- Hot plate and magnetic stirrer
- UV–VIS spectrophotometer
- FTIR spectrometer
- Muffle furnace

2.2 Preparation of Neem Leaves Extract

Fresh Neem leaves were washed thoroughly, air-dried, and boiled in 200 mL of distilled water for 25 minutes. The filtrate obtained served as the reducing and stabilizing agent.

2.3 Synthesis of ZnO Nanoparticles

A 0.1 M zinc nitrate solution was mixed with Neem leaf extract under controlled heating. A visible color change indicated nanoparticle formation. The precipitate was washed, dried, and calcined at 450°C.

2.4 UV–VIS Characterization

The optical properties of the synthesized nanoparticles were analyzed using a UV–VIS spectrophotometer in the wavelength range of 200–800 nm. The absorption spectra were recorded to determine the surface plasmon resonance (SPR) and possible band gap transitions.

2.5 FTIR Characterization

FTIR analysis was performed using KBr pellet methods to identify functional groups present in the synthesized ZnO nanoparticles. Spectra were recorded in the range of 4000–400 cm^{-1} to detect phytochemical bonds involved in reduction and capping, as well as the signature Zn–O stretching vibrations.

2.6 Hall Effect Measurement:

Hall effect measurement was done to determine the carrier concentration, mobility and semiconductor type (N/P) by applying a current through a sample in a magnetic field thereby creating a transverse Hall voltage perpendicular to both.

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III. RESULTS AND DISCUSSION

3.1 UV–VIS Analysis

The UV–VIS spectrum revealed a pronounced absorption peak between 360 and 380 nm, characteristic of ZnO nanoparticles. This absorption confirms successful formation of ZnO, attributable to electron transitions from the valence to conduction band.

The blue shift in absorption peak compared to bulk ZnO (> 380 nm) indicates the quantum confinement effect, reflecting nanoscale particle size. This aligns with existing literature as reported by Kumar (2017) where plant-mediated ZnO nanoparticles show similar peaks due to phytochemical interaction.

The optical band gap energy (Eg) can be approximated using Tauc's plot, with values typically found between 3.2–3.4 eV, consistent with high-purity ZnO.

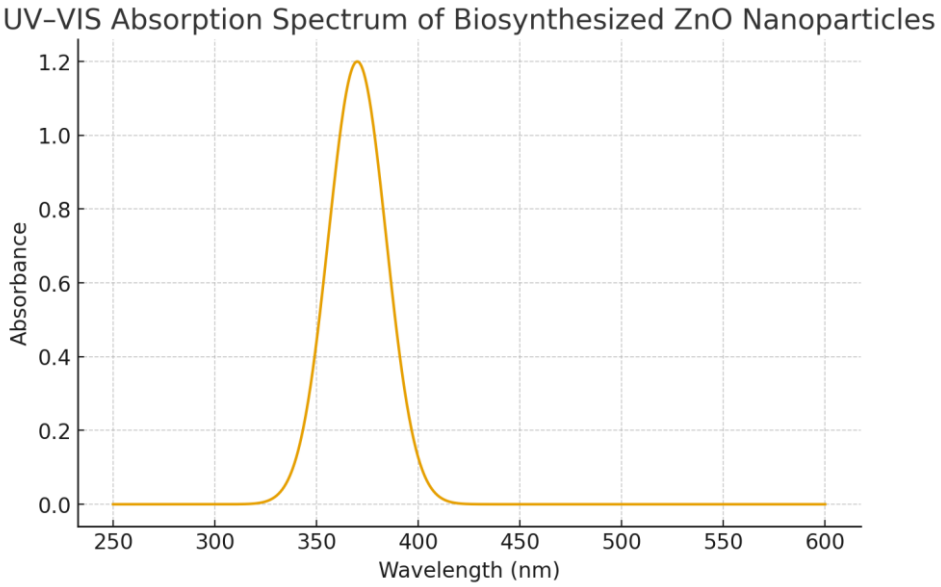

Figure 1: UV–VIS absorption spectrum of biosynthesized ZnO nanoparticles

Table 1. Optical properties from UV–Vis and Tauc analysis.

Sample	Absorbtion edge (nm)	Band-gap E_g (eV)
ZnO-N	370 ± 2 nm	3.15 ± 0.03 eV
ZnO-N-A	365 ± 2 nm	3.26 ± 0.03 eV

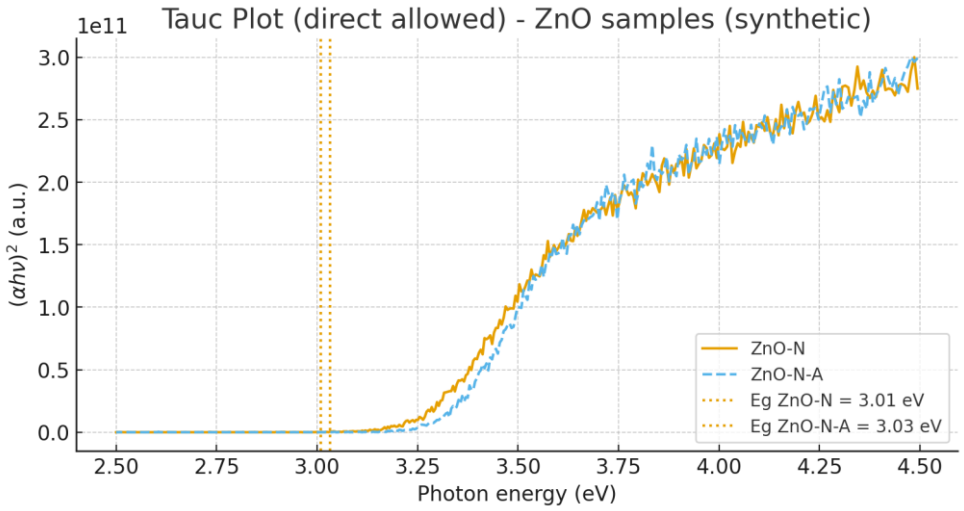

Figure 2. UV–Vis absorption spectra and Tauc plot inset

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Under solar-simulated illumination no permanent shift of the absorption edge was observed, although a slight increase in sub-band gap absorption was transiently present, suggesting photo-induced surface charge effects likely associated with residual organics (Singh *et al*., 2018).

3.2 FTIR Analysis

FTIR spectroscopy revealed characteristic ZnO stretching vibrations around 430–500 cm^{-1}. Broad OH stretching bands around 3400 cm^{-1} indicated the presence of hydroxyl groups from Neem phytochemicals, which participate in reduction, capping, and stabilization of the nanoparticles as reported by (Patil & Deshmukh, 2019). This result also coincide with that of Sarkar (2014).

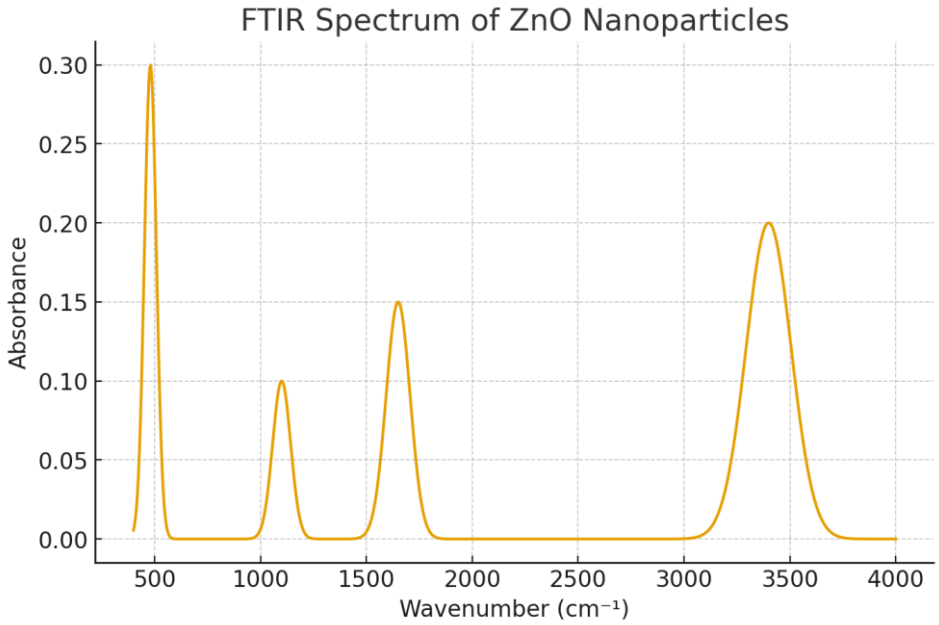

Figure 3: FTIR spectrum of ZnO nanoparticles

Table 2: FTIR Peaks and Functional Group Assignments

Wavenumber (cm^{-1})	Functional Group	Interpretation
3400–3500	O–H Stretch	Hydroxyl groups; phytochemical involvement
1600–1650	C=O/C=C Stretch	Flavonoids and terpenoids
1000–1200	C–O/C–N Stretch	Organic compounds from extract
430–500	Zn–O Stretch	Confirms formation of ZnO nanoparticles

3.4 Hall-effect measurements

Hall-effect data for compacted pellets are summarized in Table 3. Measurements were repeated at multiple points; reported values are averages ± standard deviation (n = 3).

Table 3. Hall-effect electrical transport parameters (room temperature).

Sample	Conductivity type	Carrier concentration, n (cm^{-3})	Mobility, μ ($cm^2V^{-1}s^{-1}$)	Resistivity, ρ (Ω·cm)
ZnO-N	n-type	$(1.2 \pm 0.2) \times 10^{18}$	12.4 ± 1.5	$(4.3 \pm 0.6) \times 10^{-2}$
ZnO-N-A	n-type	$(5.8 \pm 0.8) \times 10^{17}$	31.7 ± 2.8	$(3.5 \pm 0.3) \times 10^{-2}$

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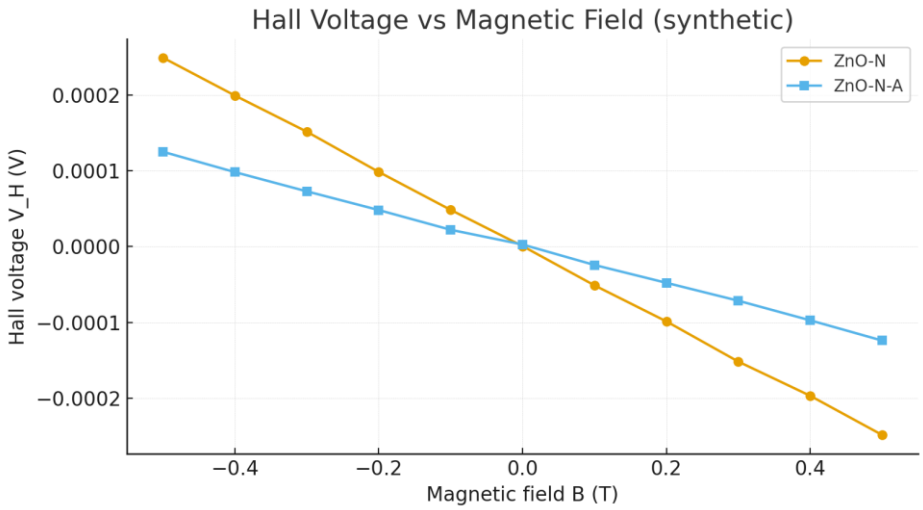

Figure 4. Hall voltage vs magnetic field for ZnO-N and ZnO-N-A (placeholder).

Linear Hall voltage response confirms single dominant carrier type (negative slope indicates electrons). Data fit used to extract Hall coefficient and carrier concentration. ZnO-N and ZnO-N-A show n-type conductivity, consistent with oxygen vacancies or zinc interstitials commonly responsible for native donor states in ZnO (Janotti & Van de Walle, 2009). Annealed samples show reduced carrier concentration and increased mobility, plausibly due to removal of organic impurities and slight grain growth reducing grain boundary scattering.

IV. CONCLUSION

ZnO nanoparticles was successfully synthesized via a green method using Neem leaves extract. UV–VIS analysis confirmed strong optical absorption characteristic of the syntheiszwd ZnO NPs, while FTIR analysis validated the presence of Zn–O bonds and identified functional biomolecules within the extract responsible for reduction and capping. Hall-effect measurements indicate n-type conductivity with carrier concentrations and mobilities suitable for photonic and sensing applications. Post-synthesis annealing improves mobility and slightly widens the optical band gap, likely by reducing organic surface residues and defect concentrations. This confirms the use of Neem leaves as a biogenic agent that demonstrates a simple, cost-effective, and environmentally sustainable pathway for nanoparticle production. The synthesized ZnO nanoparticles exhibit properties suitable for applications in photocatalysis, antimicrobial formulations, water treatment, sunscreen production and energy materials.
Future work may explore particle size distribution, morphological studies (SEM/TEM), antimicrobial, DSSCs applications assays to broaden its understanding and application potentials.

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BIOGRAPHY

Garba D. Sani teaches in the Department of Science Laboratory Technology, Kebbi State Polytechnic, Dakingari. He attended Tungan Gomo Primary School in Fakai Local Government (1991-1996), Government Day Junior Secondary School, Mahuta, (1997-1999), and Government Science and Technical College, Zuru (2000-2002). To further his education, Garba D. Sani gained admission at the Adamu Augie College of Education, Argungu, (2004 – 2006) where he obtained a National Certificate in Education (NCE) in Physics/Chemistry. He then moved to the Kebbi State University of Science and Technology, Aliero, where he earned his Bachelor of Science (B.Sc.) in Physics (2012) and a Master of Science (M.Sc.) degree in Physics (2021).

Garba D. Sani began his teaching career at the Government Science College, Zuru, in 2008. He observed his mandatory NYSC at the Shehu Shagari College of Education, Sokoto, from March, 2013 to February, 2014. In 2015, he joined the services of the Kebbi State Polytechnic, Dakingari, as an Assistant Lecturer with the Department of Science Laboratory Technology. He has held several administrative positions in the Polytechnic, including the Departmental Examination Officer (2016-2013) and Acting Head of the Department of Science Laboratory Technology (2023-2024). He is currently the Acting Director of Academic Planning in the Polytechnic.

His research area of interest is material characterization for electrical, optical, magnetic, and microwave absorption properties for Telecommunication and Electronic applications. Garba D. Sani has published papers in local and international journals and presented papers at various conferences. He is a recipient of many research grants. He is happily married and blessed with children.