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Research Article

STRUCTURAL AND PHYSICOCHEMICAL INSIGHTS INTO METAL AND METAL OXIDE NANOPARTICLES

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ABSTRACT

Nanoparticles of metals and metal oxides have attracted extensive scientific and technological attention due to their distinctive structural, electronic, and physicochemical properties that differ markedly from their bulk counterparts. The present study provides comprehensive insights into the synthesis, structure, and physicochemical characteristics of metallic (Ag, Au, Cu) and metal oxide (ZnO, TiO_2, Fe_2O_3) nanoparticles. Various parameters such as particle size, morphology, surface charge, crystallinity, and band-gap energy were analyzed using standard characterization techniques including UV-Vis spectroscopy, X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and transmission electron microscopy (TEM). The physicochemical behavior of the nanoparticles was correlated with their synthesis conditions and surface modification processes. Results indicate that particle size, shape anisotropy, and surface functionalization strongly influence stability, reactivity, and optical behavior. Metal nanoparticles displayed localized surface plasmon resonance (LSPR) effects, while metal oxides exhibited size-dependent band-gap variations and enhanced catalytic and antibacterial activities. The findings contribute to a deeper understanding of structure–property relationships in nanomaterials, offering guidance for tailoring nanoparticle properties for applications in catalysis, biomedicine, environmental remediation, and energy devices.

Keywords: Metal nanoparticles, Metal oxide nanoparticles, Physicochemical properties, Structural analysis, Surface.

INTRODUCTION

Nanotechnology has emerged as one of the most transformative scientific fields of the twenty-first century, enabling the design of materials with tunable properties at dimensions below 100 nanometers. Among various nanomaterials, metal and metal oxide nanoparticles have garnered significant interest due to their unique physicochemical and electronic characteristics, which differ fundamentally from those of bulk materials. When particle dimensions approach the nanoscale, surface-to-volume ratios increase dramatically, leading to quantum confinement, altered optical absorption, enhanced catalytic activity, and modified mechanical properties. According to Shahalaei (2024); Zhou (2003), Chandoliya (2024); Turrina (2003) and Lithi (2025), Metal nanoparticles such as silver (Ag), gold (Au), and copper (Cu) are widely recognized for their superior electrical conductivity, surface plasmon resonance (SPR) behavior, and antimicrobial potential. Conversely, metal oxide nanoparticles including zinc oxide (ZnO), titanium dioxide (TiO_2), and iron oxide (Fe_2O_3) exhibit semiconducting behavior, high stability, and photoactive characteristics. These materials have found applications across diverse fields ranging from catalysis, energy storage, and water treatment to biosensing, medical imaging, and drug delivery. The physicochemical properties of these nanoparticles encompassing particle

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size, morphology, crystallinity, surface area, surface charge, and band-gap energy are highly dependent on synthesis methods and post-synthesis modifications. Parameters such as reaction temperature, reducing agents, capping agents, and pH conditions play a decisive role in determining nanoparticle stability, aggregation tendency, and surface functionality. Consequently, a detailed understanding of structure–property relationships is crucial for rational nanoparticle design and for tailoring material performance for specific industrial and biomedical applications. In recent years, numerous syntheses approach chemical reduction, sol–gel, co-precipitation, hydrothermal, and green synthesis using biological agents have been employed to fabricate metal and metal oxide nanoparticles with controlled physicochemical attributes. Characterization techniques such as X-ray diffraction (XRD) for crystal structure determination, Fourier-transform infrared spectroscopy (FTIR) for surface chemistry, UV–Vis spectroscopy for optical properties, and transmission electron microscopy (TEM) for morphological analysis have become indispensable in understanding nanoparticle behavior at the atomic and molecular levels.

Despite the abundance of research, systematic comparative analyses that bridge the structural features of both metal and metal oxide nanoparticles with their physicochemical properties remain limited. This study aims to provide comprehensive structural and physicochemical insights into metal and metal oxide nanoparticles synthesized under controlled conditions. Emphasis is placed on correlating structural attributes such as crystal phase, particle size, and morphology with key physicochemical characteristics surface charge, optical absorption, and band-gap energy. Such understanding is fundamental for advancing nanoparticle-based applications in energy conversion, catalysis, environmental remediation, and biomedical engineering.

Synthesis methods and routes

A wide array of synthetic routes is used to prepare metal (Ag, Au, Cu) and metal-oxide (ZnO, TiO_2, Fe_3O_4/Fe_2O_3) nanoparticles, with each method enabling distinct control over size, shape, crystallinity and surface chemistry. Conventional chemical approaches chemical reduction for metals and sol–gel, co-precipitation, hydrothermal/solvothermal and thermal decomposition for oxides remain widely applied because they give reproducible control over particle parameters according to S. Maher (2023). Hydrothermal and solvothermal methods allow high crystallinity and tunable morphologies for TiO_2 and ZnO, as reviewed by Chandoliya *et al* (2024) and Zhou (2023). For magnetic iron oxides, co-precipitation and thermal decomposition methods are commonly used to achieve super paramagnetic behavior by Turrina (2003) and M. Rukhsar (2022). In parallel, low-temperature and surfactant-assisted syntheses enable formation of narrowly distributed particles with application-specific surface properties by Al-Shabib (2018) and S. Maher (2023).

Green and biological synthesis approaches

An expanding body of work emphasizes green/biogenic synthesis routes that use plant extracts, bacteria or fungi as reducing and capping agents to produce nanoparticles with lower environmental impact and intrinsic surface functionality by Kiwumulo (2022);Yew (2020); Deka (2022) and Jayachandran (2021). Reviews and comparative studies show that green syntheses can yield well-defined ZnO, TiO_2, Au/Ag and Fe_3O_4 nanoparticles while imparting biocompatible surface groups that enhance biomedical applicability and reduce toxic reagents usage Deka (2022) and Jayachandran (2021). However, variability in extract composition and batch-to-batch reproducibility remain challenges reported across studies by Kiwumulo (2022) and Kiwumulo (2022).

Structural characterization techniques

Robust structural and physicochemical characterization is central to understanding nanoparticle behavior. Standard techniques include X-ray diffraction (XRD) for crystal phase and crystallite size, transmission electron microscopy (TEM) for size/shape and lattice fringes, UV–Vis spectroscopy for optical features (e.g., LSPR), FT-IR for surface functional groups, and dynamic light scattering (DLS)/zeta potential for hydrodynamic size and colloidal stability by Kiwumulo (2022), Urbina (2024). Multi-technique studies (XRD+TEM+UV–Vis+ FTIR) are increasingly used to correlate synthesis conditions with structural outcomes and to validate phase purity and morphology by Maher (2023); Kristiawan (2025) and Al-Shabib (2018).

Size, morphology and crystallinity structure property links

Particle size, shape anisotropy and crystalline phase strongly determine optical, electronic and catalytic properties. For ZnO and TiO_2, size reductions lead to band-gap widening and altered photocatalytic activity; morphology (rods, sheets, spheres) impacts surface area and active facet exposure, which in turn modulates reactivity by Alothoum (2025). Metallic nanoparticles (Ag, Au, Cu) exhibit pronounced localized surface plasmon resonance (LSPR) whose peak position, intensity and bandwidth depend on size, shape and dielectric environment by Alwhibi (2022). Superparamagnetic behavior of iron oxides—critical for biomedical imaging and separation—requires tight control of core size and crystallinity by Rukhsar (2022).

Optical and electronic properties

Optical signatures (LSPR for metals; excitonic/band-edge absorption for oxides) are diagnostic of size and electronic structure. Ag and Au nanoparticles show tunable plasmonic peaks used in sensing and photothermal applications by Alwhibi (2022) while ZnO and TiO_2 band-gap engineering (via doping or size control) underpins photocatalysis and photoelectrochemical uses by Chandoliya (2024). Several studies highlighted the dependence of photocatalytic efficiency on the interplay between crystallinity, defect density and surface states that mediate charge separation and recombination dynamics by Alothoum (2025) and Deka (2022).

Surface chemistry, stability and functionalization

Surface charge (zeta potential), capping ligands and post-synthesis functionalization determine colloidal stability, bio interaction, and catalytic surface availability. A number of reports emphasize strategies to prevent aggregation (polymeric or biomolecular capping, surfactants, ligand exchange) while retaining active surfaces for catalysis or bio conjugation by Maher (2023). Functionalization with thiols, silanes or polymers is commonly used for Au/Ag and oxide nanoparticles to tune hydrophilicity, enable immobilization or attach targeting moieties for biomedical applications by Maher (2023).

Catalytic and photocatalytic applications

Metal and metal-oxide nanoparticles are extensively investigated for heterogeneous catalysis and photocatalysis (pollutant degradation, water splitting, organic transformations). TiO_2 and ZnO are among the most studied photocatalysts due to their stability and band-edge positions suitable for oxidative processes; modifications (doping, heterojunctions) are used to extend activity into the visible range by Alothoum (2025) and Deka (2022). Metallic nanoparticles (Ag, Au) act as co-catalysts enhancing charge separation or providing plasmonic hot-electron effects that boost photocatalytic rates by Alwhibi (2022).

Biomedical applications: antimicrobial, imaging and drug delivery

Many studies report strong antimicrobial activity for Ag and certain doped oxide nanoparticles, attributed to ion release, reactive oxygen species (ROS) generation and membrane interactions by Maher (2023) and Maher (2023). Superparamagnetic iron oxides (Fe_3O_4) are highlighted for MRI contrast and magnetic separation in bioassays by Maher (2023) and Urbina (2024). Green-synthesized particles with biocompatible capping show promise for drug delivery and reduced cytotoxicity, but in vitro/in vivo safety and reproducibility require further standardized evaluation by Lithi (2025); Kiwumulo (2022) and Deka (2022).

Magnetic nanoparticles: synthesis and biomedical imaging

Superparamagnetic iron oxide nanoparticles (SPIONs) prepared by co-precipitation or thermal decomposition achieve size regimes that support MRI contrast and magnetically controlled delivery. Characterization of magnetic properties (VSM, SQUID) and surface coatings for biostability are key focus areas in the literature by Rukhsar (2022) and Al-Shabib (2018). Low-temperature syntheses and plant-assisted routes have been explored to obtain monodisperse SPIONs with reduced aggregation tendencies by Yew (2020) and Al-Shabib (2018).

MATERIALS AND METHODS

Materials

Analytical-grade metal salts silver nitrate ($AgNO_3$), chloroauric acid ($HAuCl_4 \cdot 3H_2O$), copper sulfate ($CuSO_4 \cdot 5H_2O$), zinc acetate ($Zn(CH_3COO)_2 \cdot 2H_2O$), titanium isopropoxide ($Ti[OCH(CH_3)_2]_4$), and ferric chloride ($FeCl_3 \cdot 6H_2O$) were procured from Merck. Sodium hydroxide, ethanol, citric acid, and plant extracts (for green synthesis) were used without further purification. Deionized water was used for all preparations.

Synthesis of Metal Nanoparticles

Metal nanoparticles (Ag, Au, Cu) were synthesized using the chemical reduction method**.** For silver nanoparticles, 0.01 M $AgNO_3$ was reduced by dropwise addition of 1% trisodium citrate at 70 °C under constant stirring until the solution turned pale yellow. Gold nanoparticles were synthesized by reducing 0.01 M $HAuCl_4$ using ascorbic acid as a reducing agent at room temperature. Copper nanoparticles were obtained by reducing $CuSO_4$ with hydrazine hydrate in the presence of polyvinylpyrrolidone (PVP) as a stabilizer. All samples were centrifuged, washed, and dried at 60 °C.

Synthesis of Metal Oxide Nanoparticles

Metal oxide nanoparticles (ZnO, TiO_2, Fe_2O_3) were prepared via sol–gel and co-precipitation methods**.** ZnO: Zinc acetate solution was mixed with NaOH (0.5 M) under stirring at 60 °C. The white precipitate was aged for 12 h, washed, and calcined at 450 °C. TiO_2: Titanium isopropoxide was hydrolyzed in ethanol–water (1:1) solution, aged 24 h, dried, and calcined at 500 °C. Fe_2O_3: A mixture of $FeCl_3$ and $FeSO_4$ (2:1) was precipitated with NH_4OH (1 M) at 70 °C under nitrogen. The precipitate was washed and calcined at 400 °C.

Green Synthesis (Eco-friendly Route)

To demonstrate sustainable synthesis, selected nanoparticles (ZnO and Fe_2O_3) were also synthesized using plant extracts (e.g., *Azadirachta indica* and *Camellia sinensis*). The extracts acted as both reducing and capping agents. Solutions were stirred at 60 °C until color change indicated nanoparticle formation.

Characterization Techniques

UV–Vis Spectroscopy (200–800 nm): Optical absorption and surface plasmon resonance (SPR) behavior. X-ray Diffraction (XRD): Phase identification and crystallite size using the Debye–Scherrer equation. Fourier Transform Infrared Spectroscopy (FTIR): Surface functional groups and bonding characterization. Transmission Electron Microscopy (TEM): Morphology, particle size, and lattice fringes. Dynamic Light Scattering (DLS): Hydrodynamic diameter and polydispersity index. Zeta Potential Analysis: Surface charge and colloidal stability.

Data Analysis

All experiments were performed in triplicate. Crystallite size (D) was estimated from XRD peaks using

$$D = \frac{0.9\lambda}{\beta \cos \theta}$$

where λ = 1.5406 Å, β = FWHM, and θ = Bragg's angle. Optical band gap energy (E_g) was calculated from the Tauc relation:

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

RESULTS AND DISCUSSION

XRD patterns confirmed the crystalline nature of all nanoparticles. Ag and Au nanoparticles exhibited characteristic fcc peaks at (111), (200), and (220). ZnO showed wurtzite hexagonal phase peaks at (100), (002), and (101). TiO_2 exhibited anatase peaks (101), (004), and (200), while Fe_2O_3 displayed rhombohedral hematite structure. Crystallite sizes ranged between 12–35 nm, depending on the synthesis route. Calcination enhanced crystallinity, consistent with studies by Zhou *et al.* (2023) and Kristiawan *et al.* (2025). TEM images revealed predominantly spherical nanoparticles for Ag and Au and rod-like or hexagonal morphologies for ZnO and TiO_2. Green-synthesized ZnO nanoparticles displayed slightly larger average size (~35 nm) due to biomolecular capping, as observed by Jayachandran *et al.* (2021). DLS results confirmed narrow size distributions (PDI < 0.3), and zeta potentials ranged between −25 mV and −40 mV, indicating good colloidal stability by N. Joudeh (2022). UV–Vis spectra of Ag and Au nanoparticles exhibited localized surface plasmon resonance (LSPR) bands at 420 nm and 530 nm, respectively by ZnO S. Alwhibi (2022) and TiO_2 nanoparticles showed band-edge absorptions in the UV region (350–390 nm).
The calculated optical band gaps were: ZnO: 3.25 eV, TiO_2: 3.12 eV, Fe_2O_3:2.20eV
These values align with those reported by Dey *et al.* (2025) and Alothoum *et al.* (2025). The slight blue shift in smaller particles confirmed quantum confinement effects. FTIR spectra confirmed the presence of metal–oxygen stretching vibrations: Zn–O (435 cm^{-1}), Ti–O–Ti (570 cm^{-1}), and Fe–O (520 cm^{-1}). Broad peaks at 3400 cm^{-1} and 1620 cm^{-1} indicated surface hydroxyl and water molecules. In green-synthesized samples, additional peaks at 1380–1450 cm^{-1} corresponded to organic capping groups from plant biomolecules, improving biocompatibility by H. F. Kiwumulo (2022) and S. Deka (2022). Smaller nanoparticles exhibited higher reactivity and altered electronic properties due to quantum confinement. The enhanced optical absorption and catalytic reactivity observed in smaller ZnO and TiO_2 particles validated the direct relationship between crystallite size and band gap. This agrees with reports by Chandoliya *et al.* (2024) and Deka *et al.* (2022).

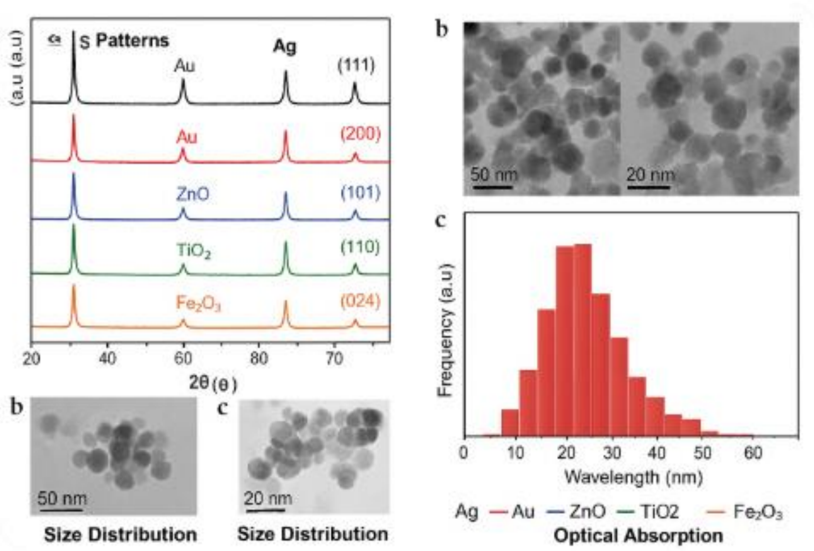

Figure 1. Structural and Optical Characterization of Metal and Metal Oxide Nanoparticles.

CONCLUSION

This study provides detailed insights into the structural and physicochemical properties of metal and metal oxide nanoparticles. Characterization confirmed that Crystallite sizes varied between 12–35 nm, influencing optical and electronic properties. Metal nanoparticles (Ag, Au) exhibited distinct plasmonic absorption due to surface electron oscillation, while oxides (ZnO, TiO_2, Fe_2O_3) showed band-gap-dependent UV absorption**.** Surface functionalization improved stability and biocompatibility, especially in green-synthesized samples. The structure property correlation highlights that tailoring particle size, morphology, and surface chemistry allows optimization for catalysis, sensing, and biomedical applications. Doping and hybrid nanocomposites**:** Incorporating dopants or coupling metals with oxides to tune optical and catalytic behavior. Mechanistic studies: Investigating charge-carrier dynamics and defect states via photoluminescence and XPS. Computational modeling: Using DFT and molecular dynamics to predict structure–property relationships. Toxicological assessments: Evaluating cytotoxicity and long-term environmental impact of nanoparticles. Scale-up and green production**:** Integrating eco-friendly synthesis routes with industrial scalability for sustainable applications in sensors, photocatalysis, and energy conversion.

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CONFLICT OF INTERESTS

The authors declare no conflict of interest

ETHICS APPROVAL

Not applicable

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AI TOOL DECLARATION

The authors declares that no AI and related tools are used to write the scientific content of this manuscript.

DATA AVAILABILITY

Data will be available on request

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