

## Synthesis and Characterization of CuO Nanoparticles for Photocatalytic Dye Degradation

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### ABSTRACT

The structural, morphological, and optical characteristics of the produced CuO nanoparticles are thoroughly understood in this work. X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier transform infrared (FTIR) spectroscopy, and UV-visible (UV-Vis) spectroscopy were used to effectively and thoroughly analyze copper oxide (CuO) nanoparticles. The XRD analysis gave insight of crystal structure of all the compositions. The XRD analysis provide an average crystallite size (D) determined by the Debye-Scherrer equation. The XRD investigation verified the development of a pure monoclinic crystalline phase. The surface morphology was shown by SEM micrographs, which showed that quasi-spherical nanoparticles with some agglomeration were present. The FTIR analysis lead to presence of functional group and bonds. The creation of the metal oxide was confirmed by the FTIR spectra, which revealed distinctive vibrational modes associated with Cu-O bonding. The Ultraviolet visible spectroscopy was done to know the optical properties of prepared samples under the increasing temperature conditions. The Tauc's plot was used to calculate the optical band gap energy, and the UV-Vis absorption spectrum showed a clear absorption peaks, underscoring its prospective uses.

**Keyword:** XRD, FTIR, SEM, UV- Vis, Agglomeration, Band Gap

### Introduction

Nanostructures that measure up to 100 nanometers in every dimension are called nanoparticles. Nanoparticles have a size and a surface that can be changed which

makes them especially useful in many areas. Nanoparticles have a large surface area compared to their volume, which changes how they behave. The exact size and shape of a nanoparticle directly affect how it reflects light. These physical features also decide how easily a nanoparticle can move into living cells. The charge on a nanoparticle's surface is another factor that controls how the nanoparticle interacts with its surroundings. This includes how the nanoparticle contacts cells and whether it can be harmful, to biology. Many studies show that nanoparticles are used in medicine, food and medical tests. Their flexibility lets them do jobs from carrying drugs to fighting germs. In short the physical and chemical traits of a nanoparticle decide how well it works in any task [1].

## Classification

Inorganic

Carbon based

Organic

### Inorganic Nanoparticles:

The group of particles comprises nanoparticles that originate from organic waste material, including agricultural waste and kitchen waste. The nanoparticles in this case contain carbon and are classified according to the physical properties and process of synthesis.

### Carbon based Carbon Dots and Nanocomposites

Carbon Dots and Their Nanocomposites: This type comprises carbon nanoparticles with fluorescence properties (less than 10 nm). They are synthesized from organic waste material such as fruit peels, agricultural waste, and other forms of biomass. The different sub-types in the group include graphene quantum dots, carbon quantum dots, and carbonized polymer dots. The integration of carbon dots with metal or polymer results in carbon dots nanocomposites[2].

### Organic nanoparticles:

Organic nanoparticles are nanoscale systems made up of only organic substances like lipids, proteins, and polymers and are different from particles derived from waste carbon. These nanoparticles have been employed in drug delivery and biomedicine and are of various types:

Micelles are the nanoparticles formed by amphiphilic molecules, resulting in spherical structures with hydrophobic cores. The benefits that these nanoparticles exhibit include hydrophilicity, nontoxicity, simple synthesis, controlled drug delivery, and biomedical applications [3]. Liposomes are spherical structures with aqueous cores surrounded by one or more layers of lipids. Liposomes are biodegradable, can transport both hydrophilic and hydrophobic drugs, and highly stable [4]. Dendrimer nanoparticles are highly branched tree-like macromolecules of a definite structure with adjustable sizes and surface properties for drug delivery[5, 6]. Polymeric nanoparticles are solid colloidal particles synthesized with biodegradable synthetic and natural polymers. These nanoparticles are easily synthesized, stable for storage, and biocompatible [7]. Solid lipid nanoparticles (SLN) are particles made up of high

melting point lipids stabilized with surfactants and have the advantage of high stability, controlled release, and low toxicity [8]. Protein complex nanoparticles are the nanoparticles made from protein materials that are biodegradable, non-toxic, and have good surface properties [9]. The description of nanoparticles is dominated by the dependence of their surface, optical, magnetic, mechanical and thermophysical properties on size. Due to the large increase in surface-to-volume ratio ( $3/r$ ), 20% and 90% of atoms in nanoparticles at 10 nm and 1 nm belong to the surface. As a result, many dangling bonds arise because of the presence of a large amount of under coordinated atoms that have high energy and chemical reactivity, making nanoparticles excellent catalysts and leading to the tendency to aggregation. The surface charge, composition and crystallographic orientation may affect the stability of nanoparticles as well as their interaction with living cells and proteins (protein corona) [10]. The optical properties of nanoparticles are characterized by surface plasmon resonance, which depends on the size and shape, and collective oscillations of electrons give the impression of color: gold is red and silver is yellow [11, 12]. The semiconductor nanoparticles have size-dependent optical properties, which include the quantum confinement effect and allow emitting visible light: the smaller particles are blue, and the bigger ones are red, which may be used in displays and imaging [13]. From a magnetic perspective, nanoparticles can display superparamagnetism at sizes below 20 nm, enabling the control of their motion via an external magnetic field for photothermal therapy and heating, which can also be used for targeted cancer treatment with no permanent magnetization of the tissue [14]. Mechanically, such nanoparticles can demonstrate mechanical properties superior to those of bulk materials: for instance, carbon nanotubes are 100 times stronger and tougher than steel while weighing 1/6 as much, and smaller particle size can be associated with increased hardness in materials (Hall-Petch effect) [15]. As for other properties, thermal ones are also determined by the reduced size of nanoparticles: they possess lower melting points (at 2–3 nm Au size, melting temperature is 300–400°C compared to 1064°C in bulk Au) and, for certain materials, demonstrate increased thermal conductivity [16].

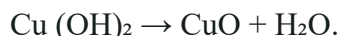
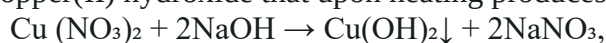
The use of copper as an antimicrobial agent dates back to ancient civilizations, and its beneficial effects have been known since 3000 BC [17]. In the present era, dental caries, among other oral infections, are major public health problems and are mainly caused by the development of pathogenic biofilms on tooth surfaces [18]. This has necessitated the development of novel approaches to effectively combat oral biofilms without being fully dependent on conventional antimicrobial agents, which are experiencing increasing difficulties of bacterial resistance [19]. Copper has gained popularity in medical [18] and dental studies because of its antimicrobial property and low toxicity [18]. The antimicrobial properties of copper occur either through copper ions [20] or through the oxidation of copper ions obtained from copper nanoparticles (1–100 nm). Moreover, the availability of copper nanoparticles makes them cheap; these nanoparticles are prepared either through natural or chemical means and readily oxidize when exposed to air or water, resulting in copper oxide nanoparticles. Copper nanoparticles, like other metal nanoparticles used in dentistry, have various nano sizes and forms, unique size distribution, and high surface area to volume ratios.

## Experimental details

Where there is no mention of something else in the article, all the chemicals that have been used in this experiment were obtained and used in their analytical grade form only. Before starting the experimental synthesis procedure all the beakers,

## Properties, Synthesis, and Uses of Chemicals and Copper Oxide

In this experimental study, copper (II) nitrate trihydrate was utilized as the copper source, sodium hydroxide (NaOH) as the precipitant, sodium borohydride as a reducing agent if needed, and polyethylene glycol (PEG) as a capping agent if needed. Copper (II) oxide or cupric oxide (CuO) is an inorganic compound that is in the form of a black or dark brown odorless powder and has a molar mass of 79.55 g/mol and a monoclinic crystalline structure. It is almost insoluble in water but dissolves in acid media, producing copper salts; its density is 6.3 g/cm<sup>3</sup>. It is quite stable in room conditions but starts decomposing at a temperature of 1,326°C. The oxide is basic and reacts with acids to form copper salts and water. It may be reduced to copper metal by hydrogen and carbon monoxide. The material is a p-type semiconductor with a small band gap of 1.2–1.7 eV and has antiferromagnetic properties at low temperatures. The oxide may be obtained by a reaction of copper (II) nitrate with sodium hydroxide to yield copper(II) hydroxide that upon heating produces copper oxide and water,



It finds applications in medicinal such as antibacterial creams and wound-healing, environmental applications for dye removal and toxin removal from water, energy generation in batteries and solar cells, sensors to detect gases like CO and glucose, and industrial applications as a pigment for ceramics and glass. Some of its important characteristics include being a p-type semiconductor, antimicrobial against bacteria and viruses, catalyst for oxidation reactions, environmentally friendly and economically viable in comparison to metal oxides, and antiferromagnetic at low temperature.

## Materials and Characterizations of CuO Nanoparticles

CuO nanoparticles prepared were analyzed by XRD, SEM, FTIR, and UV-Vis analysis methods. XRD was used to confirm the crystalline monoclinic phase and crystallite sizes from Cu K $\alpha$  radiation at  $2\theta = 20 - 80^\circ$ . Surface morphology, particle sizes, and agglomeration were investigated by SEM after gold coating. FTIR analysis (4000 - 400 cm<sup>-1</sup> KBr pellet) was done to confirm Cu-O bond at 400 - 600 cm<sup>-1</sup>. Optical absorption and band gap were performed by UV-Vis (200 – 800 nm).

## Results and Discussion

### XRD Analysis

In the current section the structural analysis of copper oxide nanoparticles via XRD will be performed; this type of crystallographic study is crucial and inevitable for structural elucidation of any solid material. XRD analysis is of crucial significance for investigation of nanomaterials, as it gives vital information about the crystal structure,

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phases, lattice parameters, unit cell size, crystallite size, micro-strain and in general crystalline quality of the material, all of which are strongly correlated with synthesis conditions and strongly determine physical and chemical properties of the synthesized material. The diffraction pattern of the copper oxide nanoparticles, prepared through synthesis process, was obtained via XRD within suitable  $2\theta$  range with monochromated  $\text{CuK}\alpha$  radiation ( $\lambda = 1.5406 \text{ \AA}$ ). The obtained diffraction pattern was analyzed carefully, and the diffraction peaks were indexed, comparing them with reference diffraction patterns from International Centre for Diffraction Data (JCPDS/ICDD) database. Such an analysis allowed to identify the exact copper oxide phase(s) in the sample and check the phase purity of the material. The data on peak positions, intensity ratios, and full-width at half-maximum have been used for the estimation of lattice parameters, unit cell volume, and extent of crystallinity. The mean crystal size has been calculated based on the Debye-Scherrer formula  $D = K\lambda/\beta\cos\theta$  ( $K = 0.9$ ,  $\beta$  is FWHM in radian,  $\theta$  is Bragg's angle). The micro-strain effects have been assessed by the integral breadth method and Williamson-Hall plots. The results are discussed in relation to the correlation between the properties of the samples and the synthesis conditions like the precursor concentration, pH, reaction temperature, and calcinations. The chart below represents XRD spectra of copper oxide nanoparticle synthesized through four different conditions, (i) to (iv). This was achieved within a  $2\theta$  range of  $20^\circ$  to  $60^\circ$ . All four samples have peaks at  $32^\circ$ ,  $39^\circ$ ,  $49^\circ$ ,  $54^\circ$  and  $58^\circ$  corresponding to the monoclinic  $\text{CuO}$  phase. Sample (i) has wide and weak peaks. On the other hand, curves (ii) and (iii) have sharper and more pronounced peaks than curve (i). Lastly, curve (iv) has the most sharp and intense peaks of all the four samples.

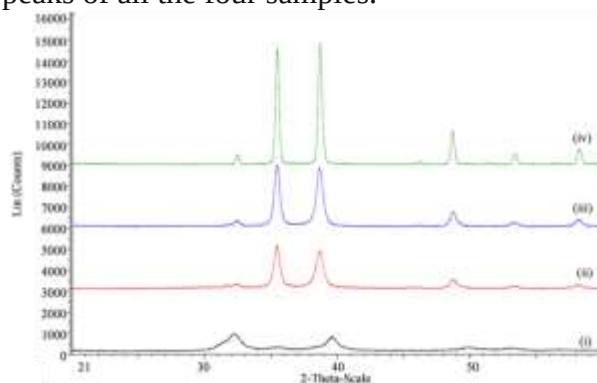


Figure 1: XRD analysis of Copper Oxide ( $\text{CuO}$ )

It is thus evident that the crystallinity of  $\text{CuO}$  increases and crystallite size increases. The systematic decrease in FWHM from (i) to (iv) thus implies an increase in the crystallite size and this is quantified through the Debye-Scherrer equation. There are no extra peaks implying purity of the sample while the trends imply synthesis condition significantly affects structural quality, crystallite size and crystallinity of the  $\text{CuO}$  nanoparticles.

### Surface morphology (SEM) Analysis

Surface morphology and microstructure of the synthesized copper oxide were analyzed using Scanning Electron Microscope (SEM). Good quality micrographs

were captured at an accelerating voltage of 15 kV and a  $\times 10,000$  magnification, having a scale bar of 1  $\mu\text{m}$ . The imaging was done through the use of CRL UOP secondary electron detector with high-vacuum and room-temperature conditions to avoid any charging, beam damage, and contamination effects. The micrographs showed the shapes of the primary particles, the textures of the surfaces, the grain boundaries, roughness, distance between the particles, crystallographic facets, and agglomeration or dispersion degree. The scale bar helped in estimating the sizes of the particles, their homogeneity, and distribution semi-quantitatively. But SEM can only provide morphological details of the particles. It cannot tell about the ratio of copper to oxygen, the purity of the element, its oxidation state, and crystallographic phases. Thus, the identity of the compound can only be determined based on the known process and precursors used for synthesis, and the confirmation is needed from EDS, XPS, or Raman Spectroscopy. No image editing or any kind of post-capture processing was done in order to maintain the integrity and objectivity of the data.

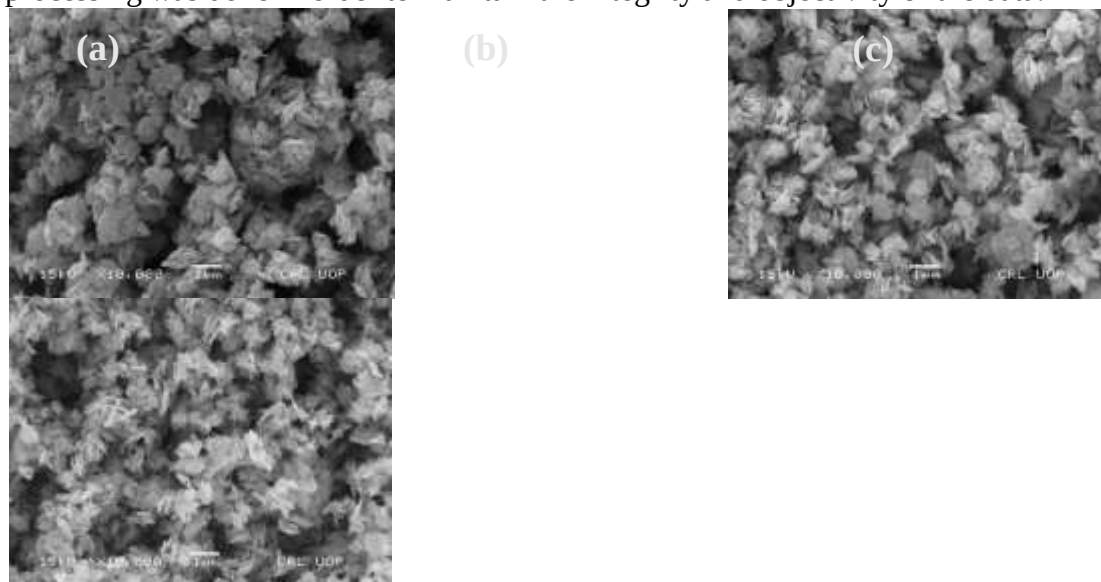


Figure 2: SEM (a, b, c) analysis of Copper Oxide (CuO)

Table1: Scanning Electron Microscope (SEM)

| PARAMETER            | VALUE/ DESCRIPTION                 |
|----------------------|------------------------------------|
| Instrument           | Scanning Electron Microscope (SEM) |
| Material analysed    | Copper Oxide                       |
| Accelerating voltage | 15kv                               |
| Magnification        | *10000                             |
| Scale bar            | 1um                                |
| Detector type        | Secondary electron (SE)-CRL UOP    |

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|                                 |                                                |
|---------------------------------|------------------------------------------------|
| Operating condition             | High vacuum, room temperature                  |
| Imaging mode                    | Surface topography                             |
| Morphological features revealed | Particle shape, surface texture, agglomeration |

## FTIR Analysis

In this subsection, surface chemical characterization of copper oxide nanoparticles via FTIR spectroscopy will be described. FTIR is useful for molecular structure, chemical bonding and functional groups of materials. FTIR analysis of nanoparticles plays a crucial role because their surface chemistry, which includes surface functional groups, metal ion coordination, adsorption, interaction with stabilizers/capping agents etc., largely affects colloidal stability, reactivity and applicability in photocatalysis, sensing, biomedicine and environmental applications. FTIR spectra were acquired in the range from 4000 to 400  $\text{cm}^{-1}$  in KBr pellet/ATR. Every band was identified on the basis of its comparison with reference and literature data, with particular emphasis being put on Cu–O vibrations below 700  $\text{cm}^{-1}$ , which indicate formation of copper oxides; the exact position of bands depends on phase (either CuO or  $\text{Cu}_2\text{O}$ ), size of particles and crystallinity. In addition, the spectrum was checked for O–H stretching band at about 3400  $\text{cm}^{-1}$ , water adsorption band at about 1630  $\text{cm}^{-1}$  and potential organic impurities such as C–H stretch vibration ( $\sim 2920\text{--}2850$   $\text{cm}^{-1}$ ), carbonyl stretching vibration ( $\sim 1700$   $\text{cm}^{-1}$ ), and C–O stretch vibration ( $\sim 1100$   $\text{cm}^{-1}$ ).

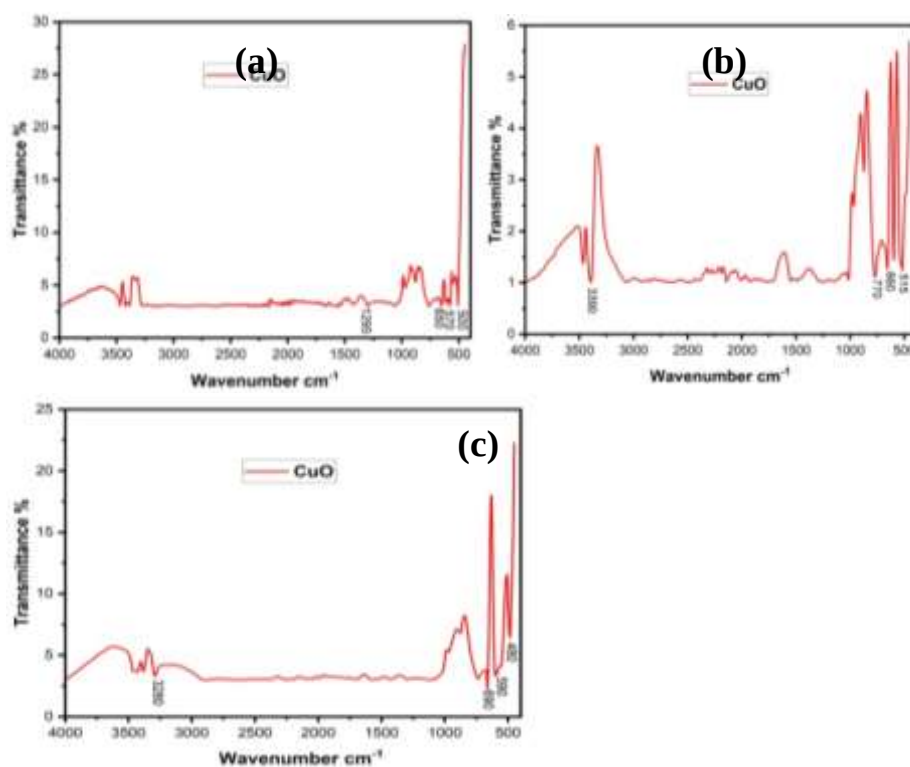


Figure 3: FTIR (a, b, c) of CuO

The three FTIR spectra of the synthesized copper oxide nanoparticles within 4000 to

400  $\text{cm}^{-1}$  range. In all the three graphs, there are wide bands of O-H stretching from 3400 to 3280  $\text{cm}^{-1}$  as well as H-O-H bending at 1630-1654  $\text{cm}^{-1}$ , which proves the presence of surface hydroxyl groups and absorbed water, a shift of O-H stretching to 3280  $\text{cm}^{-1}$  in the third graph shows the presence of stronger hydrogen bonding. C-H bands at 2939  $\text{cm}^{-1}$  in the second and third graphs show some impurities of organic origin, whereas the bands in the range of 1100-700  $\text{cm}^{-1}$  result from vibrations of the lattices and adsorbed molecules such as carbonates. In the first two graphs, there is a strong band of Cu-O stretching at  $\sim 500$ -540  $\text{cm}^{-1}$ , which proves that copper oxide in phase pure form has been synthesized. In the third graph, however, there are two bands of Cu-O at  $\sim 590$  and  $\sim 500$   $\text{cm}^{-1}$ , where the latter band dominates, which shows that mostly copper oxide with little amounts of copper suboxide, possibly due to crystallite size, has been synthesized.

## UV-Vis Analysis

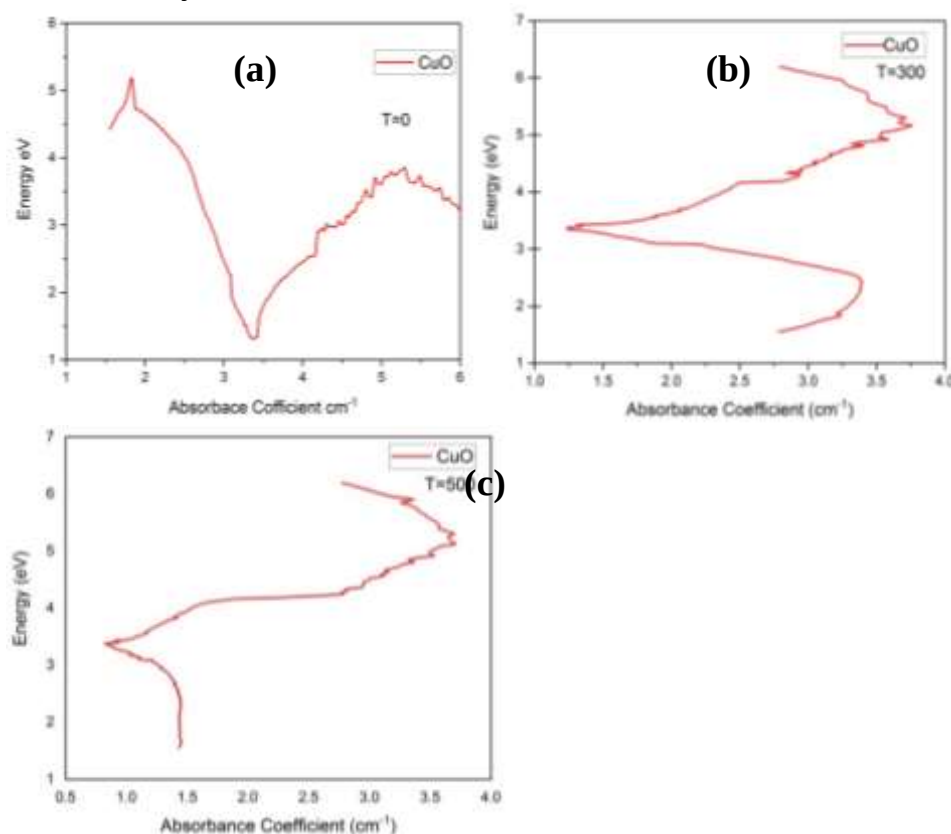


Figure 4: UV visible analysis (a, b, c) of Copper Oxide (CuO)

The UV-Vis absorption spectrometry method was applied to study the optical properties of the Copper Oxide (CuO) samples prepared at 0 °C (Sample 1), 300 °C (Sample 2), and 500 °C (Sample 3). With the increase in the temperature of synthesis, there is a noticeable trend in the absorption spectra. UV visible spectroscopy is the procedure whereby the optical properties of the produced nanomaterial were analyzed. The energy bandgap was estimated using the Tauc plot method. The optical properties made it possible to determine whether the material was suitable for use in any scientific or technological application.

## Conclusion

This research work used the green chemical precipitation technique to synthesize copper oxide (CuO) nanoparticles. Copper nitrate trihydrate ( $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ ) was the precursor, sodium hydroxide (NaOH) the precipitant, and polyvinyl alcohol (PVA) the stabilizing agent; the obtained nanoparticles were heat treated at 500 °C. X-ray diffraction (XRD), scanning electron microscopy with energy-dispersive X-ray spectroscopy (SEM-EDX), and Fourier-transform infrared spectroscopy (FTIR) techniques were used to characterize the synthesized CuO nanoparticles. XRD results indicated that the CuO particles had a monoclinic structure corresponding to JCPDS 48-1548 with nanocrystallite size, but not  $\text{Cu}_2\text{O}$  and metallic copper. SEM results depicted mostly spherical and irregular particles, while EDX and elemental analysis confirmed copper and oxygen as major elements of CuO. FTIR indicated the presence of Cu-O stretching bands below  $700\text{ cm}^{-1}$ , surface O-H bands near  $3400\text{ cm}^{-1}$ , adsorbed water at  $1630\text{ cm}^{-1}$ , and weak C-H stretching bands. Applications of these materials might include the use of antibacterial agents, gas sensors, energy storage, catalysis, and wastewater removal through adsorption of these materials. Drawbacks associated with these samples include their inconsistency in terms of crystalline nature, presence of organic impurities, wide particle size distribution, lack of optical and thermal analysis, and lack of application evaluation. Further investigations must vary the precursor concentration, pH, temperature and calcinations.

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