Structural, morphological and optical properties of CuO nanoparticles prepared through chemical method.

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Abstract: The Cupper oxide (CuO) nanoparticles (NPs) prepared by co-precipitation method. The XRD patterns showed that the synthesized CuO NPs exhibits monoclinic structure. The FESEM image showed that, the synthesized CuO NPs were formed nanoflake like structure. The Chemical compositions were identified by EDAX spectra. The Cu-O stretching vibrations were observed by FT-IR spectra located at 655 cm^{-1} for CuO NPs respectively. UV-Vis absorption spectra, the absorption edge peak observed at 224 nm for CuO NPs samples. The PL spectral measurements revealed that the broad emission bands observed, due to cupper interstitials (Cu_i) and oxygen vacancies (V_O).

Keywords: CuO; XRD; UV; FTIR; PL;

1 Introduction

Nanotechnology gained much attention for its vital pioneering role in manipulating materials at the atomic and molecular levels to dramatically alter the product properties. Materials reduced to the nanometric scale display significantly different properties compared to what they display at the macroscale or microscales. Because of their unique properties, nanomaterials are widely used in a variety of applications. Small amounts of nanoparticles can play a vital role in developing the properties of materials. Nanoparticles are becoming more and more important day by day as they play a beneficial role in a wide variety of scientific fields.

In recent years, nanostructures of transition metal oxides have gained a great attention from material scientists and engineers due to their different properties compared with the corresponding bulk counterparts, which in turn provides promising applications in various fields of technology. Preparation of high quality nanostructures of defined, controllable size and morphology is a critical requirement in order to develop nanodevices or other different applications for catalyst, sensing, pharmacy [1–7], and so on.

CuO, categorized into transition metal oxide group, is a p type, narrow bandgap semiconductor. It has monoclinic structure and many interesting characteristics: super thermal conductivity, photovoltaic properties, high stability, and antimicrobial activity. Due to such exclusive properties, CuO can be used in many technological fields, for example, active catalyst [1], gas sensor [4, 6], high efficiency thermal conducting material [7], magnetic recording media [8], with very good selectivity, or solar cell applications [9].

In the present investigation, Copper oxide (CuO) nanoparticles (NPs) prepared by co-precipitation method. The synthesized CuO NPs were characterized by X-ray diffraction studies, Field Emission Scanning Electron microscope, Energy dispersive X-ray spectroscopy, Fourier Transform infrared spectroscopy, UV-Vis spectroscopy, and Photoluminescence spectroscopy studies carried out.

2 Materials and Method

2.1 Synthesis

Copper (II) nitrate hexahydrate (AR), and NaOH (AR) were used as precursor materialsfor the synthesis of CuO NPs.

A 0.1 M amount of copper nitrate solute was completely dissolved in deionized water. 0.8 M amount of NaOH solution was added in drops to the aqueous copper nitrate solution under constant magnetic stirring for 30 min under room temperature followed by heating process for 5 hours at 80 ˚C. The resulting solution is reflexed at room temperature for a day. So obtained residual was washed several times with deionized water and ethanol. The resulted black precipitate was dried at 120 ˚C for 1 hour. The obtained CuO samples in powder form were annealed at 700 ˚C in air for 5 hours and used for further studies.

2.2 Characterization techniques

The CuO NPs were characterized by X-ray diffractometer (model: X'PERT PRO PANalytical). The diffraction patterns were recorded in the range of 20º - 80º for the CuO samples where the monochromatic wavelength of 1.54 Å was used. The samples were analyzed by Field Emission Scanning Electron Microscopy (Carl Zeiss Ultra 55 FESEM) with EDAX (model: Inca). FT-IR spectra were recorded using Perkin-Elmer spectrometer. The UV-Vis-NIR spectrum recorded in the wavelength range 200-1100 nm by using Lambda 35. Photoluminescence spectra were measured using Cary Eclipse spectrometer.

3 Results and discussion

3.1 X-ray diffraction studies

The X-ray diffraction results of the synthesized CuO NPs are shown in Figure. 1. The characteristic diffraction peaks are obtained at angles (2θ) of 32.13, 35.13, 38.33, 45.91,48.33, 53.09, 57.09, 61.12, 65.82, 67.69, 72.01, and 745.74 corresponding to crystal plane (-110), (002) , (111), (-202), (020), (202), (113), (-311), (-113), (311) and (004) respectively. The standard diffraction peaks could be indexed to a monoclinic CuO phase (space group $C_{2/c}$) in accordance with the standard (JCPDS card no: 45-0937) [10-13].

The lattice constants 'a' and 'c' of monoclinic structure can be calculated by usingthe relation

$$\frac{1}{d^2} = \frac{1}{\sin^2\beta}\left(\frac{h^2}{a^2} + \frac{k^2\sin^2\beta}{b^2} + \frac{l^2}{c^2} - \frac{2hl\cos\beta}{ac}\right)$$

The calculated lattice constant a = 4.56 Å, b = 3.48 Å and c = 5.15 Å for synthesized CuO NPs are very closely related to the standard values are a = 4.679 Å .b = 3.431 Å, c = 5.136 Å. The average crystallite size of the NPs was calculated after appropriate background corrections from X-ray line broadening of the diffraction peaks using Debye Scherrer's formula [14].

$$\text{Average crystallite size } D = \frac{0.9\,\lambda}{\beta \cos\theta}$$

where λ =1.54060 Å, β is the angular peak width at half maximum in radius and θ is Bragg's diffraction angle. The average crystalline size is estimated as 28 nm for CuO NPs

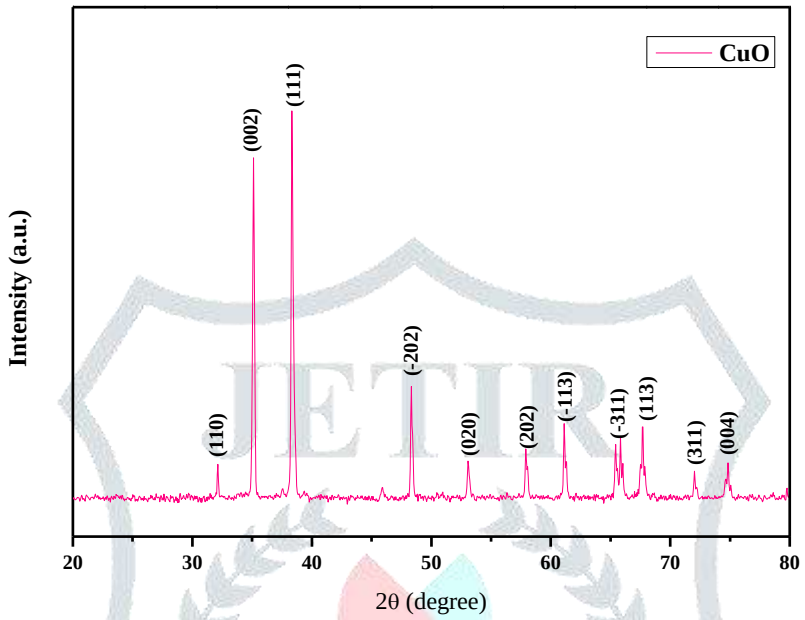

Figure 1 XRD pattern of CuO NPs

4.2 FESEM analysis

The FESEM images of the synthesized CuO nanoparticles is shown in Figure.2 (a-b). The synthesized CuO NPs exhibits nanoflake like structure and average thickness of the nanoflake 35 nm. The exact growth mechanism of obtained nanoflake CuO NPs can be explained as follows. The CuO crystallites polar faces are capable to absorb ions from the solution, in contrary ion adsorption along c axis are restricted. Afterwards, the growth along this axis declines, which is due to the cause of flaky particles formation.

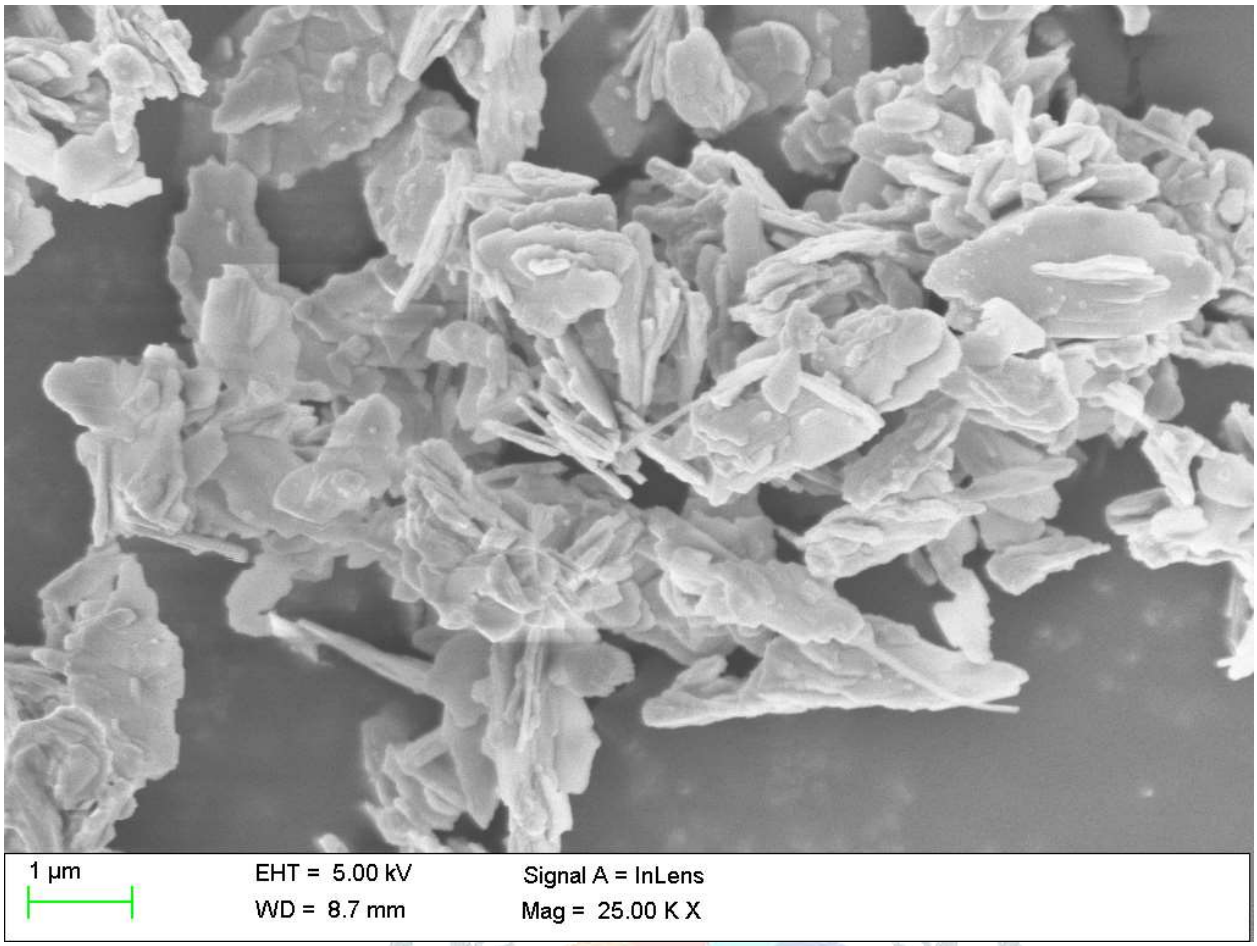

Figure 2a FESEM lower magnification image of CuO NPs

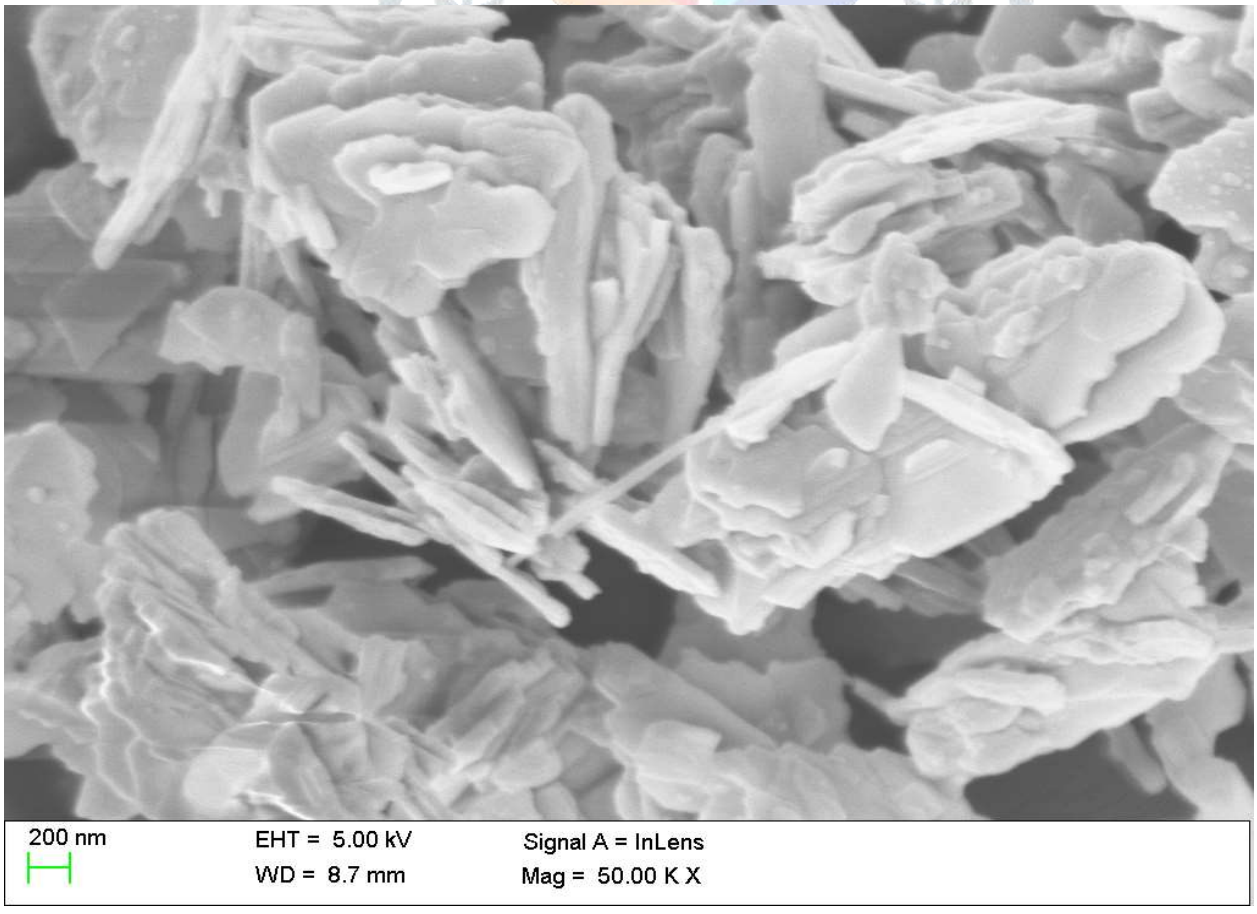

Figure 2b FESEM higher magnification image of CuO NPs.

4.3 Energy Dispersive Analysis X-ray (EDAX) Studies

The Elemental composition analysis of the CuO NP sample are confirmed by using EDAX is shown in Figure.3. The elemental composition values are given in Table 1. In the pure CuO NPs samples, the chemical compositions of Cu and O atomic percentage are observed at 50.65% and 49.35 % respectively.

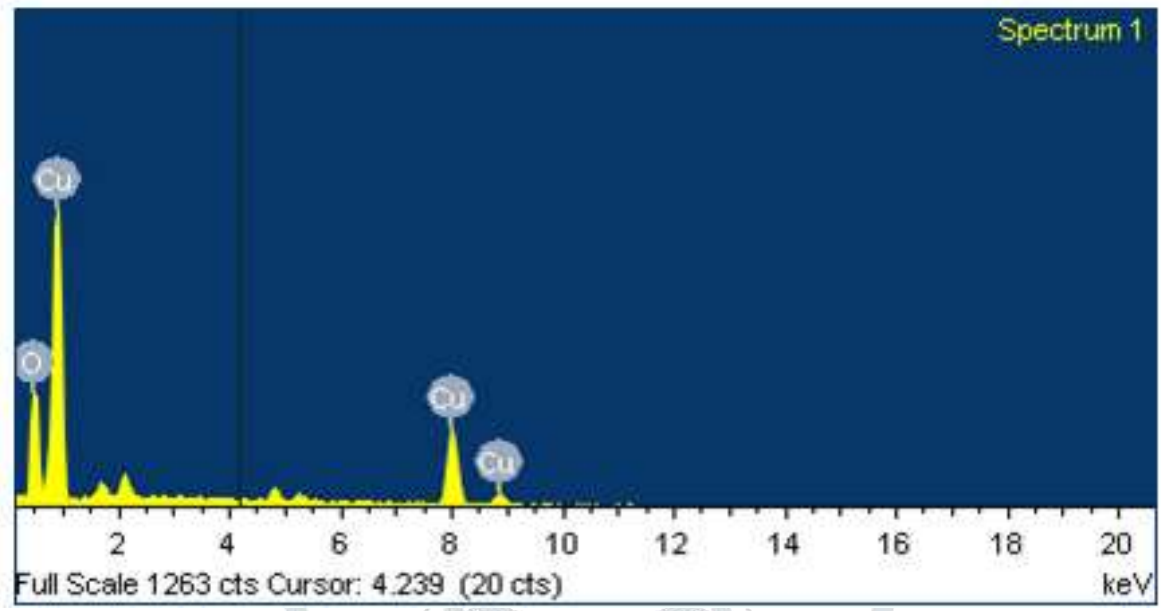

Figure 3 EDAX spectra of CuO NPs

Table – 1 Chemical composition of CuO NPs

Element	Weight%	Atomic%
Oxygen	20.54	50.65
Cupper	79.46	49.35
Total	100.00	

4.4 FTIR spectroscopic studies

Figure 4 shows that, FTIR spectra recorded in the range of 400-4000cm^{-1}forCuO NP samples. The peaks in the range of 3020-3650cm^{-1} correspond to vibrational mode of –OH stretching [13]. The sharp band centered at 3430 cm^{-1} for CuO, which due to –OH stretching of surface absorbed water molecules. The -OH bending vibration is observed at 1642 cm^{-1} for CuO NPs. The absorption peaks in the range of 400-850 cm^{-1}are associated with Cu-O, O-Cu-O and Cu-O-Cu lattice vibrations [14]. However, the Cu-O stretching bands are observed at 655 cm^{-1}for CuO NPs.

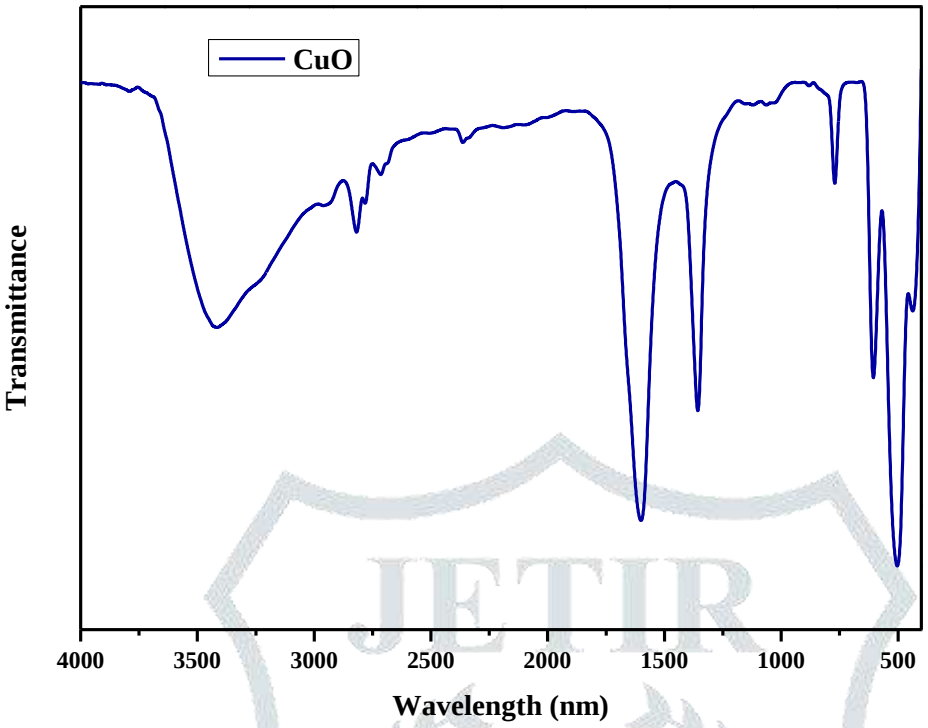

Figure 4 FTIR spectra of CuO NPs

3.2. UV-Vis spectroscopic studies

Figure 5 shows that, the UV-Vis absorbance spectral analysis of as-prepared CuO NPs. The excitonic peaks are observed at 224 nm for CuO NPs samples. This can be attributed to the photo excitation of electrons from the valence band to the conduction band.

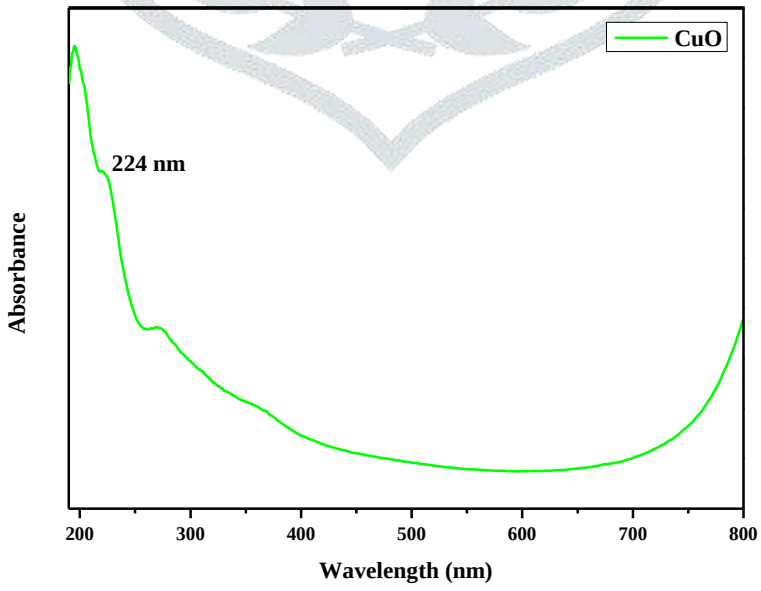

Figure 5 UV-Vis absorbance spectra of CuO NPs

4.6 Photoluminescence spectroscopic studies

The photoluminescence spectra of the CuO NPs recorded with the excited wavelength of 250 nm as shown in Figure. 6. The emission spectra of the CuO NPs sample having three peaks at 340 nm, 394 nm and 458 nm. These bands are three Near Band Edge emission and blue emissions respectively. The NBE emissions are 340 and 394 nm attributed to the recombination between electrons in the conduction band holes in the valence band [15]. The blue emission is 458 nm attributed is due to the level emission such as oxygen vacancies and Cu interstitials.

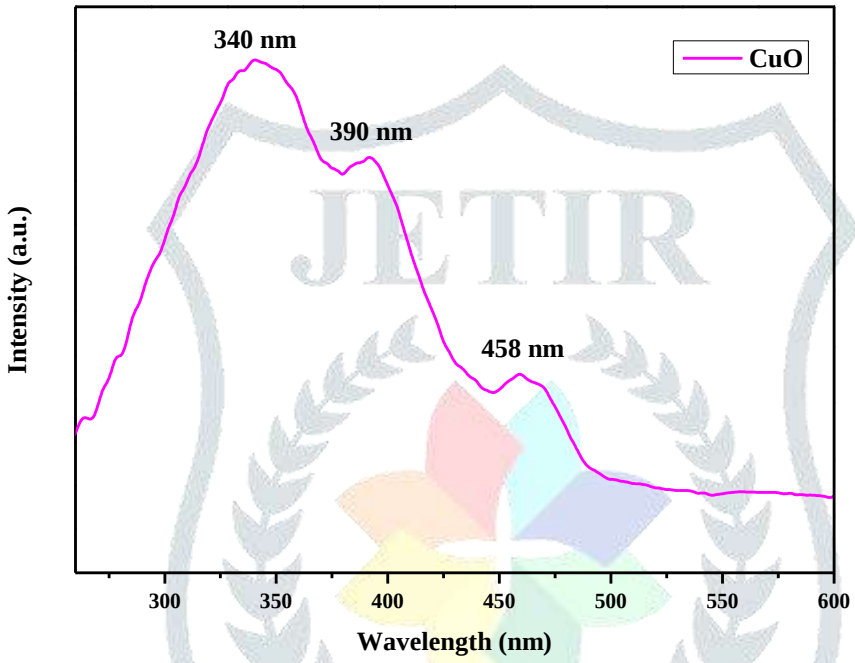

Figure 6 PL spectra of CuO NPs

Conclusion

In summary, CuO nanoparticles were prepared by co-participation method. The X-ray diffraction pattern synthesized CuO NPs exhibits monoclinic. The average crystallite sizes are calculated at 28nm for CuO NPs. The FESEM images showed that the CuO NPs formed nanoflake like structure. Elemental compositions were obtained from EDAX spectra. Metal characteristics peaks were identified using FTIR. The UV-Visible absorption edge peak observed at 224 for CuO NPs. In the PL spectra, UV and visible luminescence of CuO, due to its defects or vacancies, which was generally located on the surface of the NPs.

Author Contributions:

Dr. CB carried out the preparation of the nanoparticles and executes the physical characterization studies and contributed to the main text of the manuscript. Mr. MAR checked the scientific information and flow of the text to maintain a better readability. Further this research work is not funded by any agency.

Compliance with ethical standards:

Conflict of interest: The authors declared that they have no conflict of interest.

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