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Structural and Optical Properties of Co doped CdS Nanoparticles Synthesised by Chemical Method

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Abstract:

Constructed using the sol gel technique, the CdS nanoparticles contain cobalt. Scientists used X-ray diffraction (XRD) analysis to determine the properties of the particles they collected. The structural characterization results demonstrate the synthesis of impurity-free, Co-doped CdS nanoparticles in a single phase. We have shown and discussed the UV-VIS spectrophotometer-recorded optical absorption spectra of the doped sample in the 350–800 nm wavelength range. According to the Tauc relationship, the energy band gap is 2.46 eV. Potentially useful uses for co-doped CdS include photocatalysis, sensors, and solar cells.

Introduction:

Nanoparticles of cadmium diselenide (CdS) exhibit a comparatively high nonlinear optical response and photocatalytic activity, making them an attractive candidate for use in nanoelectronics and other photocatalytic applications. Size, form, and dimension are key factors in determining their physical attributes because of the strong relationship between their qualities and structures. Semiconductors' optical and electrical characteristics may be fine-tuned by doping, which is crucial for semiconductors' possible uses in biotechnology, solar cells, and wavelength-controlled lasers. Magnetic ion doping of semiconductor nanoparticles may result in a novel material class called diluted magnetic semiconductors (DMSs) (Dietl, 2010). Bulk semiconductors containing Mn and Co ions have shown magnetic coupling in II-VI materials (Seong et al., 2001). There is a lot of interest in DMSs right now because of the many possible uses for them in domains like spin-based electronics, or "spintronics," as well as in the fields of magnetics, electronics, and biological labelling. Semiconducting alloys (Alsaad, 2014), semiconducting films (Santra et al., 2005), and nonmagnetic semiconductors (Ohno et al., 2000) are all examples of semiconductor devices that can benefit from spintronics, which aims to regulate electron spins for information transmission. Researchers are interested in learning more about the processes used to create nanocrystals doped with magnetic ions because of the materials' potential uses and the fact that they may exhibit new magneto-optical phenomena. The synthesisability and widespread use of CdS, an II-VI semiconductor material, make it a useful tool for both the display and teaching of new technologies (Ibid.). Additionally, by including a third element, CdS may transform into a doped semiconductor due to its high band gap of 2.42 eV. Doping CdS NCs with magnetic ions, such Mn, has been a major area of research (Ohno, 1998).

Keywords: Nanomaterials, CdS, X- Ray diffraction,Optical properties.

Experimental method:

We used the sol-gel method to synthesis CdS nanoparticles that were doped. There was no additional purification required for any of the compounds as they were all analytical grade and purchased from Sigma-Aldrich. The necessary quantity of cobalt nitrate [Co $(NO_3)_2.6H_2O$] and an aqueous solution of cadmium nitrate [Cd $(NO_3)2.4H_2O$] were mixed using a magnetic stirrer for 2 hours at 80 ^{0}C. The solution (cadmium nitrate + cobalt nitrate) was heated for 6 hours before adding a water-based sodium sulphide (Na_2S) solution drop-wise. We got a green precipitate after adding sodium sulphide solution. Centrifugation was applied for 20 minutes at 5000 rpm after the solution had been rinsed with distilled water and ethanol to eliminate any contaminants. To achieve the final co-doped CdS nanoparticles, the product was removed and placed on a ceramic petri dish. Then, it was dried in a vacuum oven set at 100˚C for 9 hours. We used a mortar and pestle to grind the dry material into a fine powder, which allowed for more accurate characterization.

Result and discussion

XRD Analysis:

The XRD analysis revealed the crystal structure of the sol-gel synthesized Co-doped Cds. Figure 1 shows the operation of a device with Cu Kα radiations (λ = 1.54 A˚) operating at 30 kV and 15 mA current within the 2θ range of 15.0 to 65.0. We indexed the XRD patterns using Powder X software. The sample's XRD pattern, as seen by Bragg reflections at diffraction angles 2θ of (25.8 0), (43.20) and (51.2 0), corresponds to the (111), (220), and (311) peaks, respectively, and has a single cubic structure (JCPDS Card No.80-6019).

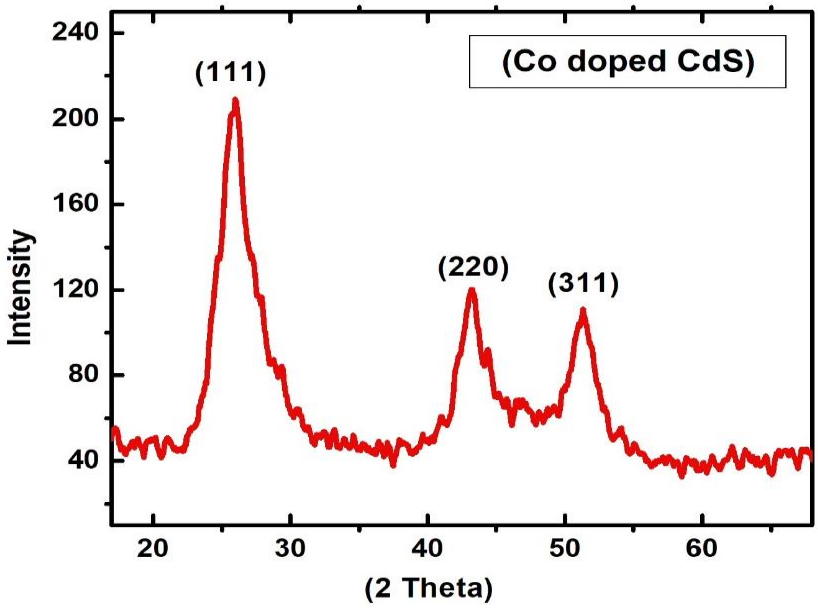

FIG.1. RXD OF Co doped CdS nanoparticles

The crystallite size calculated by using the Debye-Scherrer equation (Mahdi et al., 2018; and Mahdi et al., 2019), and found to be 25 nm by

$$D = k\lambda/ \beta \cos \theta \qquad (1)$$

"Where, D is the average crystallite size, k is constant = 0.9, λ is the wavelength of X-ray radiation (Cu Kα=1.5406 Å), β is the full width at half-maximum (FWHM), θ is the Bragg angle 2θ".

UV-Visible:

Figure (2) displays the absorption spectra of CdS nanoparticles doped with Co, measured between 300 and 800 nm. The blue shift, as seen in the absorption peaks, is due to the quantum confinement effect and is different from the bulk material.

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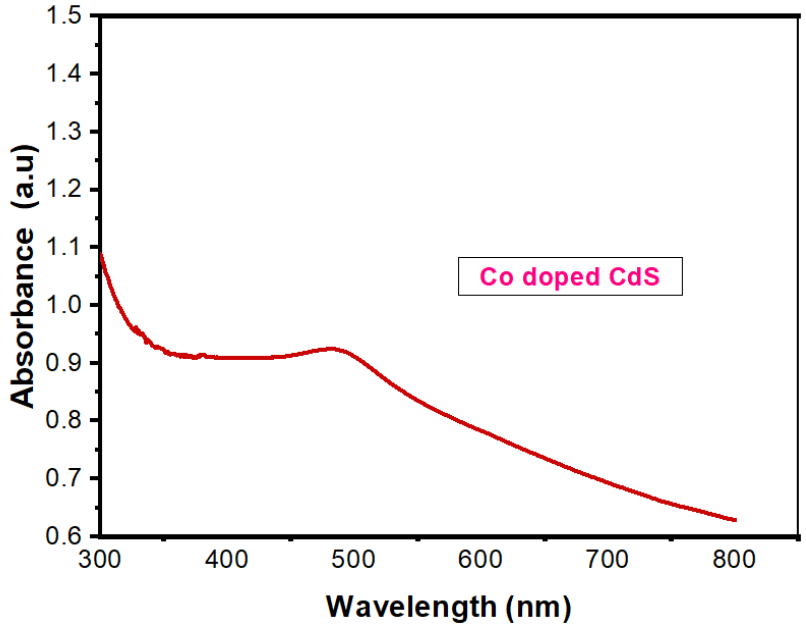

FIG. 2. Absorbance spectra as a function of wavelength for Co doped CdS

The optical band gap was determining by the Tauc relation (Mahdi et al, 2017):

$$\alpha h\nu = A(h\nu - Eg)^n \qquad (2)$$

The equation (2), as shown in Figure 3, can take on various values (2, 3, etc.), and the result is 2.46 eV, "where α is the absorption coefficient, Eg is the optical energy gap, hν is the photon energy, A is a constant, and n is the index".

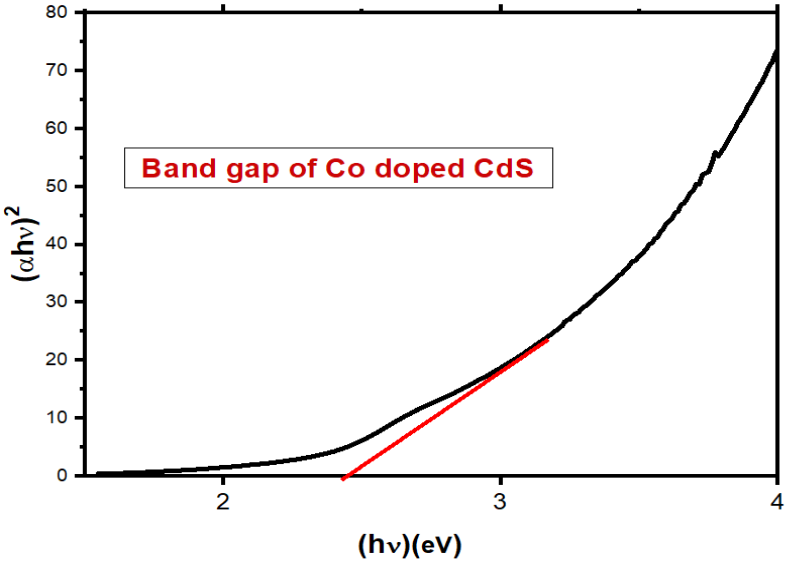

FIG.3. Band Gap of Co doped CdS

FTIR Spectroscopy:

We utilized a Perkin-Elmer Model of FTIR spectrophotometer from Iraq, which operates in the 4000 - 400 cm^{-1} range, to analyse the samples as shown in fig (4). We combined a 5 mg sample with 100 mg of KBr and compressed it into a pellet using a hydraulic press. All FT-IR spectra analysis required the KBr pellet procedures.

We may analyse the vibrational and functional groups in the CdS system by looking at the room temperature FTIR spectra of Co doped CdS NPs. Because the -OH group demonstrates the stretching vibration of the absorbed water on the CdS surface, a significant absorption peak at 3419 cm^{-1} is seen. The water molecule's OH bending vibration causes the absorption band at 1623 cm^{-1}.At 1105 cm^{-1}, the absorbed CO_2's C-O stretching vibration generates a strong peak. (Giribabu

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et al, 2013)The O-C=O asymmetric stretching vibrations are responsible for the absorption peak at 1391 cm^{-1}. Doped CdS particles have a stretching vibration peak at 630 cm^{-1} (Lazell et al, 1999).

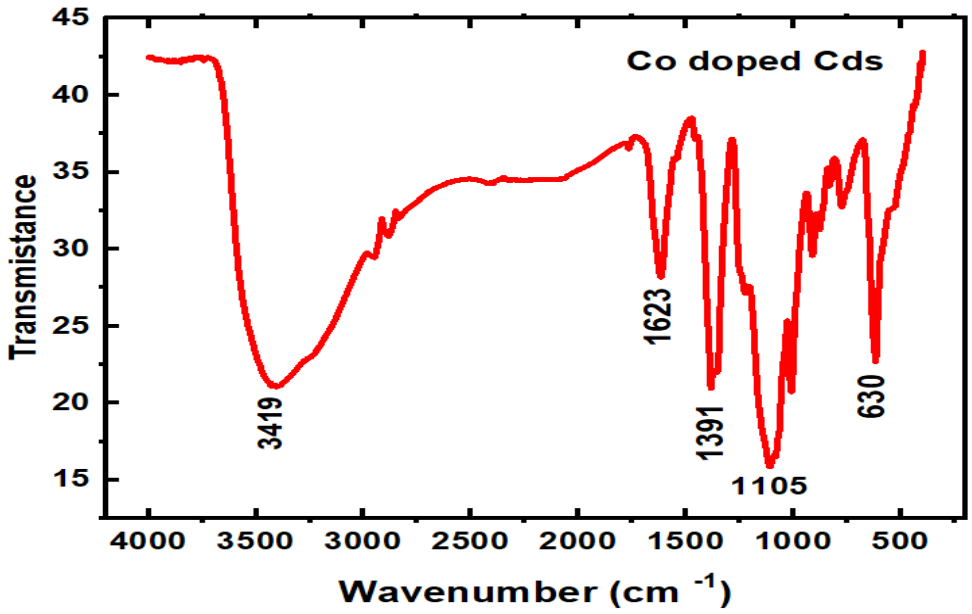

FIG 4. FTIR spectra of Co doped CdS

Conclusions:

We have successfully synthesized CdS nanoparticles that were doped by sol gel method. The confirmation of nanoparticle structure of Co doped CdS was completed through XRD data which shows the presence of all the main peaks. The optical band gap measures as 2.46 eV for Co doped CdS. The coordination of oxygen ions surrounding the CdS was confirmed by FTIR analysis.

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