



# Nd-doped CdS nano-particles: optical band gap and Urbach energy investigations

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## Abstract

CdS:Nd<sup>3+</sup> nano-particles were synthesized by chemical precipitation method and characterized by EDAX, XRD and absorption spectra and SEM imageries. XRD spectra were recorded in terms of  $2\theta$  versus counts. The particle sizes were calculated by using the strongest diffraction peak with Debye-Scherrer formula. From the XRD analysis, the average particle size of CdS:Nd<sup>3+</sup> nano-particles were found to be 1 to 50 nm. The absorption spectra, consisting of several absorption bands, have been recorded for 400–900 nm wavelength. From the absorption edge, the optical band gap and Urbach energy were computed. The concentration of Nd<sup>3+</sup> ion increases as the optical band gap and Urbach energy decreases. The presence of the high intensity peaks shows that the prepared sample were highly crystalline in nature. The obtained range of band gap is suitable for optoelectronics applications like solar cell fabrication and high frequency application.

**Keywords** CdS:Nd<sup>3+</sup> nanomaterial · XRD · Absorption spectra · Urbach energy

## Introduction

Due to their unique optical, physical, and electrical properties, semiconducting optoelectronic materials play an active role in the fabrication of a wide variety of devices. Modification of these properties of semiconductor materials depends upon the dimensions, shape, size and morphology of the material [1]. These size dependent properties of semiconductor have led scientists to focus on synthesizing nano-meter

dimensions, comparable to the Bohr radius. Such particles with Bohr radius may lead to quantum dot lasers, single electron transistors and several other biological applications [2]. Cadmium sulphide (CdS) semiconductor is superior visible light detector compared to other semiconductors [3, 4]. CdS, having a direct band gap of 2.42 eV at 300 K, possesses many useful chemical and physical properties. This leads to suitable promising applications of CdS in many devices associated with modern needs like photochemical devices, sensor devices, detector devices, opto-electronic devices, luminescence devices, solar cells and many more [4, 5]. Over the past few decades, many techniques have been reported for the synthesis of CdS nano-particles [6]. Possibility of finding new experimental methods helps to provide nano-particles at very low cost with narrow size and shape distribution. In recent years, scientists have devoted themselves in the preparation of high-quality CdS nano-particles and the study of their various properties [7]. This work aims to study the characterization of CdS:Nd<sup>3+</sup> nano-materials from its EDAX, XRD and absorption spectra and the SEM imageries. The absorption spectra were used to estimate the optical band gap and the Urbach energy.

Urbach's energy is considered as the characteristic energy which can determine the decrease of rapidity of the absorption coefficient for below band gap energy. Alternatively, it can be defined as the exponential rise in absorbance

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with energy. It essentially quantifies the sharpness of the commencement of absorption near the edge of the band. An investigation of the Urbach energy can be associated with the quantitative measure of the number of defects. So, it essentially gives an idea of the static and dynamic disorder of a semiconductor.

## Experimental details

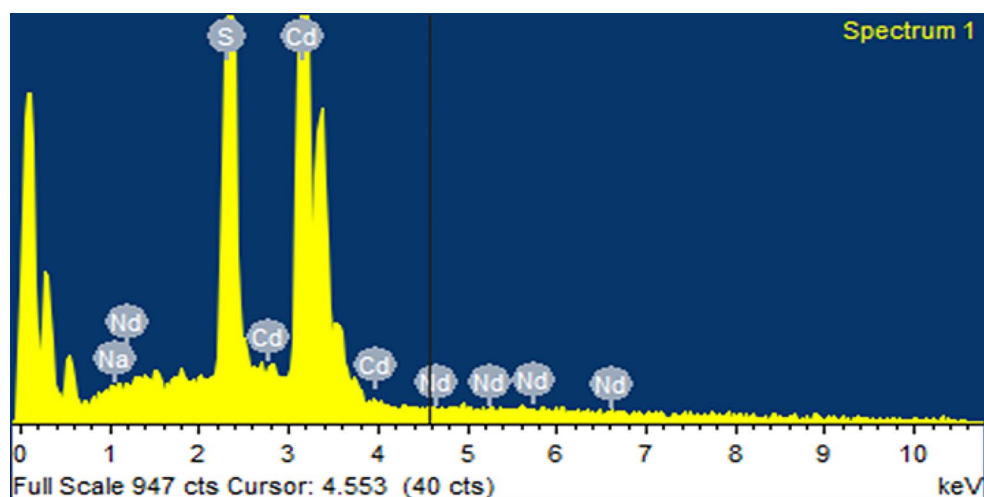
The CdS: Nd<sup>3+</sup> nano-material were synthesized by simple chemical precipitation synthesis method. This method is an inexpensive and one-step method. The chemicals, used in this study, were of analytical grade. Cadmium nitrate tetra hydrate [Cd(NO<sub>3</sub>)<sub>2</sub>·4H<sub>2</sub>O], sodium sulphide [Na<sub>2</sub>S], Diethylene glycol [DEG], ethanol [C<sub>2</sub>H<sub>5</sub>OH], neodymium chloride [NdCl<sub>3</sub>] and distilled water were used as pre-requisite material. 0.1 M of Cd(NO<sub>3</sub>)<sub>2</sub>·4H<sub>2</sub>O (50 ml) was poured in an Erlenmeyer flask. Around 20 ml of DEG was added to the Cd(NO<sub>3</sub>)<sub>2</sub>·4H<sub>2</sub>O solution with constant stirring. 50 ml of Na<sub>2</sub>S solution and different concentration (0.1, 0.2 & 0.3 mol %) of NdCl<sub>3</sub> were added drop wise with constant stirring, and the reaction was undergone for 4 h at 60°C with constant stirring. Finally, it was washed with ethanol and distilled water and dried at room temperature [8, 9]. The material was characterized by EDAX, XRD and the absorption spectra. Absorption spectra were recorded on a 2375 double beam spectrophotometer in the wavelength range from 400 to 900 nm at room temperature.

## Result and discussion

### EDAX

The representative EDAX spectrum of 0.1 mol% Nd<sup>3+</sup> ion doped CdS nano-particle is shown in Fig. 1. This spectrum

**Fig. 1** Representative EDAX spectrum of 0.1 mol% Nd<sup>3+</sup> ion doped CdS nano-particles



reveals that all the elemental abundances are present in the final composition which is taken initially. EDAX analysis justifies the elemental composition and successful incorporation [10].

### X-Ray diffraction (XRD) analysis

The X-ray diffraction (XRD) patterns of the sample are recorded with Cu K<sub>α</sub> radiation ( $\lambda = 1.5406 \text{ \AA}$ ) using a Philips XRD diffractometer. XRD was measured in terms of  $2\theta$  over the range 10–90 degrees with sampling rate of 4 deg/min. XRD pattern of CdS:Nd<sup>3+</sup> nano-particles with different concentration (0.1, 0.2 and 0.3 mol%) of Nd<sup>3+</sup> ions were synthesized and is shown in Fig. 2. All the diffraction peaks are well assigned to the hexagonal wurtzite phase of CdS when compared with standard reference (JCPDS file No. 89-2739) [11]. The presence of the high intensity peaks indicates that the prepared sample was highly crystalline in nature.

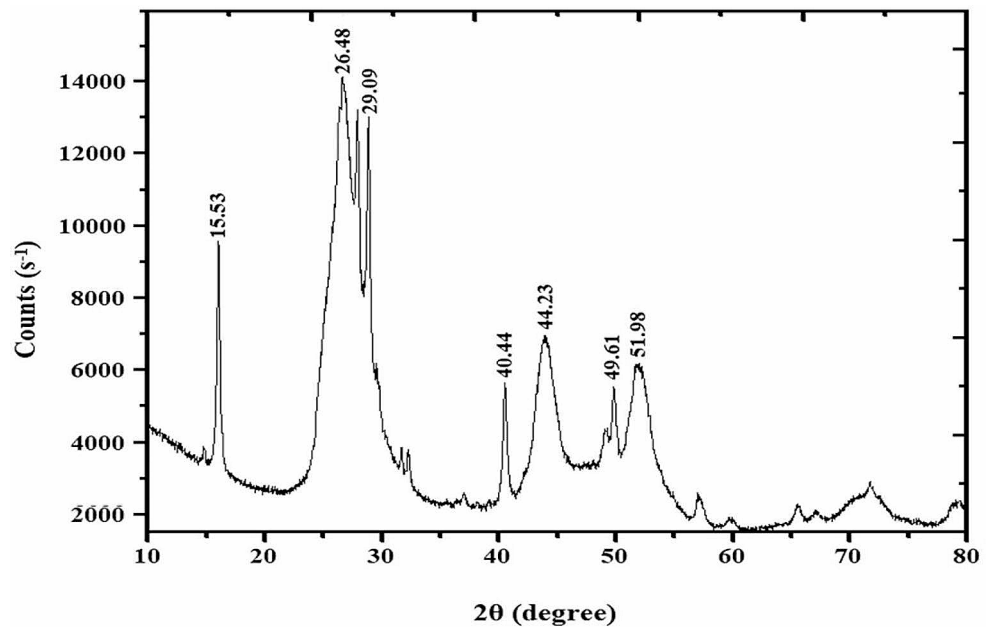
Particle sizes ( $D$ ) of CdS:Nd<sup>3+</sup> nanomaterials containing different concentration of Nd<sup>3+</sup> ions (0.1 mol%, 0.2 mol%, 0.3 mol %) were calculated using the Debye-Scherrer equation with the strongest diffraction peak. The average size of the CdS:Nd<sup>3+</sup> nano-particles was found to be in between 1 and 50 nm (Table 1).

Using the strongest diffraction peak in XRD pattern, different parameters like peak position ( $2\theta$ ), particle size ( $D$ ), full width at half maximum (FWHM) ( $\beta$ ), lattice spacing ( $d$ -value), dislocation density ( $\rho$ ), distortion parameter ( $g$ ), asymfactor, microstrain ( $\epsilon$ ) were evaluated by the Scherrer formula [12]. Table 2 represents all those evaluated parameters for 0.1 mol% Nd<sup>3+</sup> ion doped CdS nano-particles.

### Scanning Electron Microscopy (SEM)

SEM image of Nd<sup>3+</sup> doped CdS nano-particles, shown in Fig. 3, with different concentration of Nd<sup>3+</sup> ions clearly

**Fig. 2** XRD Spectra of CdS nano-material doped with 0.1% mol Nd<sup>3+</sup> ion



**Table 1** Particle size of CdS: Nd<sup>3+</sup> nano-material for different concentration of Nd<sup>3+</sup> ions along with their peak positions

0.1 mol%		0.2 mol%		0.3 mol%	
Peak Position 2θ (in deg)	Particle Size D (in nm)	Peak Position 2θ (in deg)	Particle Size D (in nm)	Peak Position 2θ (in deg)	Particle Size D (in nm)
15.53	30.51	16.04	27.93	27.94	9.12
26.48	2.51	26.65	2.73	28.80	1.0
29.09	4.47	28.84	30.54	40.49	38
40.44	20.98	40.48	23.11	43.95	5.80
44.23	9.70	51.82	4.7	49.95	27.19

**Table 2** Various parameters computed from XRD for 0.1 mol% Nd<sup>3+</sup> ion doped CdS nano-particles

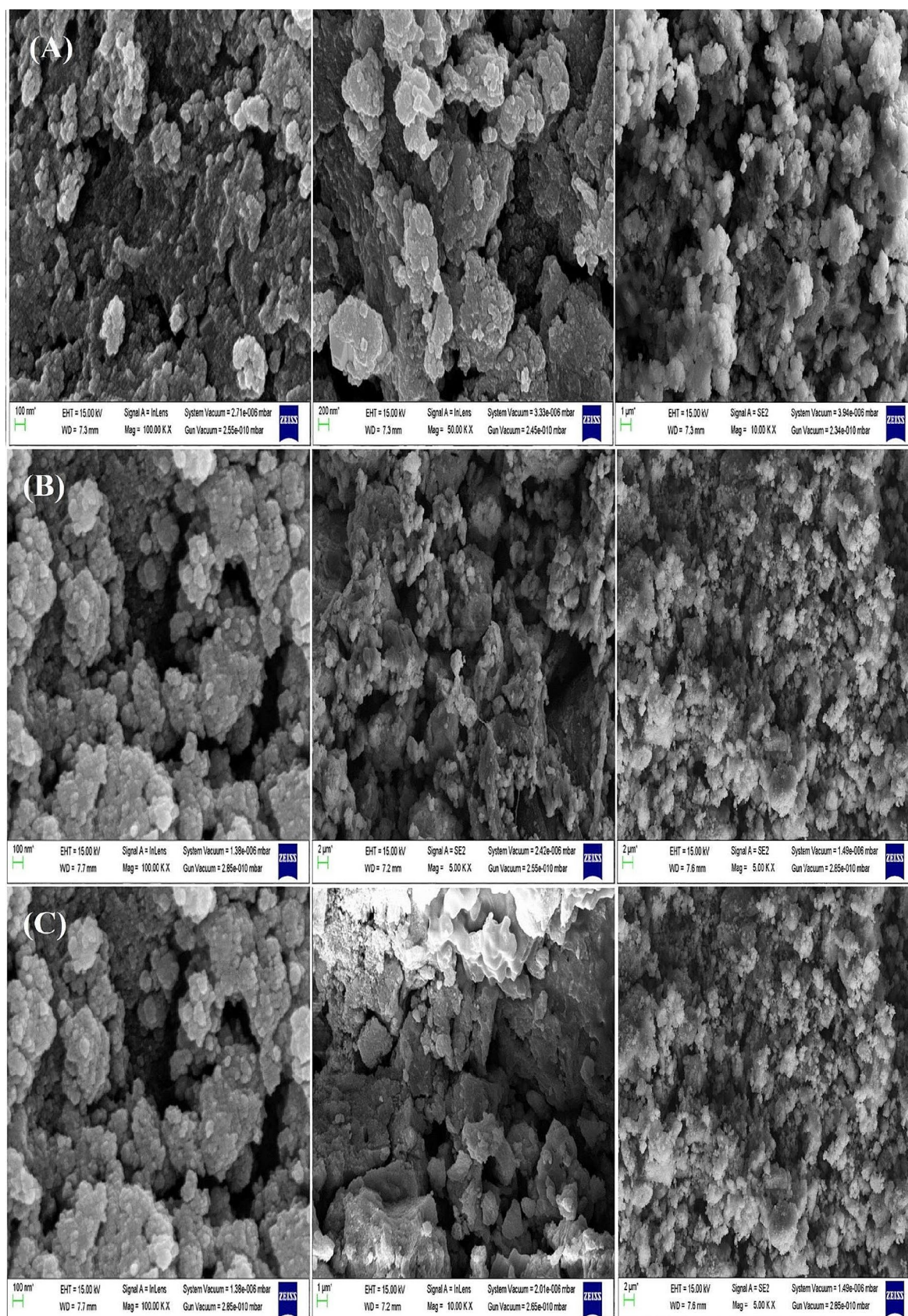
Peak position 2θ (in deg)	Particle size D (in nm)	FWHM (in deg) ( $\beta$ )	d-value (Å) observed	Dislocation density ( $\rho$ ) (in 10 <sup>15</sup> m/m <sup>3</sup> )	Distortion Parameter (g)	Asym Factor	Micro-strain ( $\epsilon$ )
15.53	30.51	0.26	1.1	1.0	1.63	1.62	0.06
26.48	2.51	3.0	0.65	149	12.29	0.95	0.72
29.09	4.47	1.83	0.60	50	6.93	0.85	0.44
40.44	20.98	0.36	0.44	2	0.97	40.50	0.08
44.23	9.70	0.76	0.37	10	1.66	49.09	0.17

indicates the formation of nano-clusters. The figure suggests that the particles are well distributed homogeneously. It indicates that a particle has the agglomeration of nano-powder [13]. The SEM images of Nd<sup>3+</sup> doped CdS nano-particles have been synthesized by simple chemical precipitation method at room temperature. The synthesized particles are nearly spherical shaped and the grain size is decreased with the increase of Nd<sup>3+</sup> ion concentration. The average grain size was analyzed to be 100 nm.

### The absorption spectra

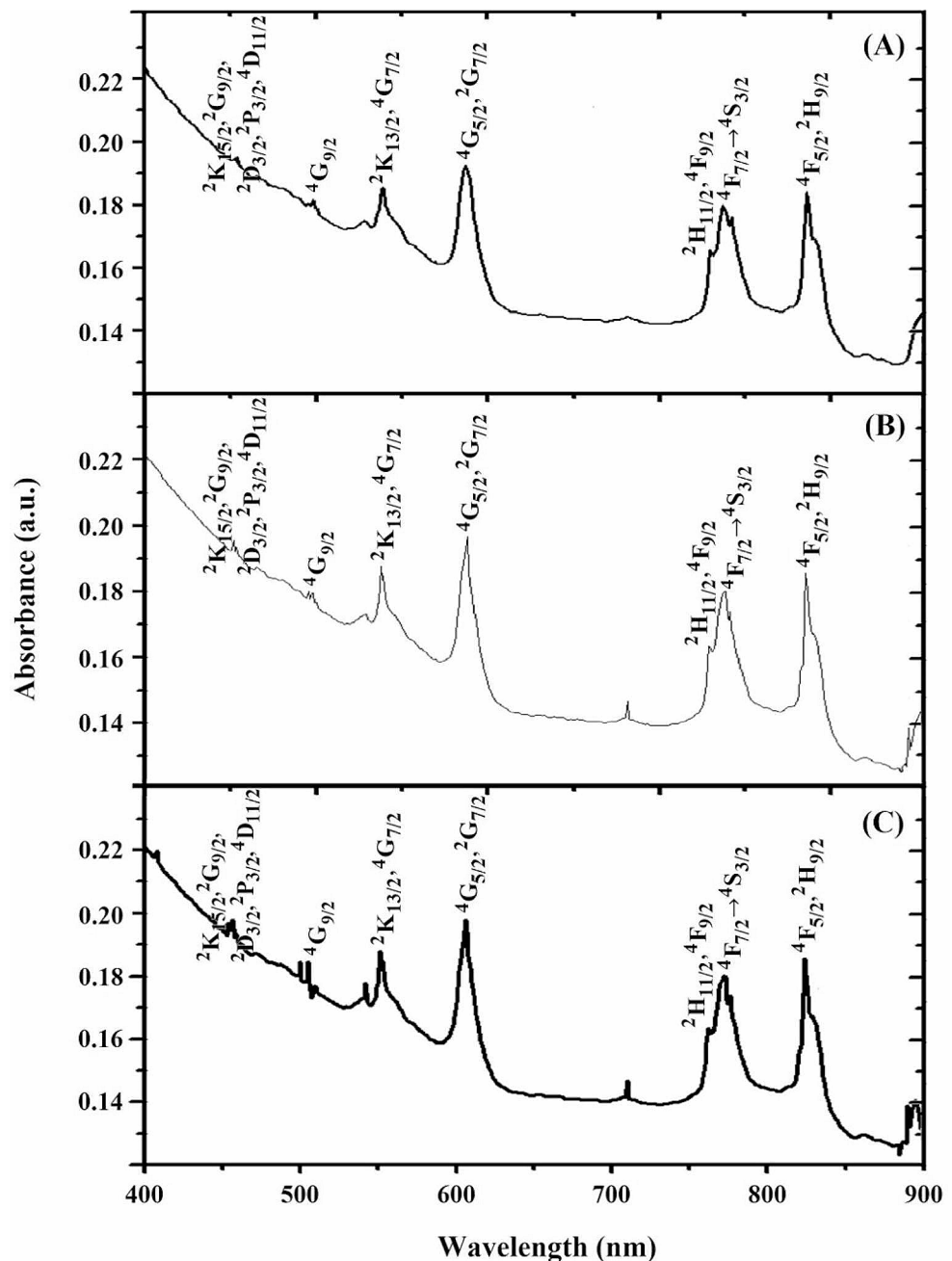
Absorption spectra of CdS:Nd<sup>3+</sup> nano-particles, consisting of several absorption bands, were recorded in the wavelength range from 400 to 900 nm at room temperature by using a UV-visible double beam spectrophotometer and is represented in Fig. 4. The peak shift in wavelengths is observed after doping of Nd<sup>3+</sup> ions. The optical absorption coefficient ( $\alpha$ ) for a sample of thickness  $t$  was computed from the absorbance  $A$ , using the following Eq. (1) [14],





**Fig. 3** SEM images of  $\text{Nd}^{3+}$  doped  $\text{CdS}$  nano-particles prepared by simple chemical aqueous precipitation method for (A) 0.1 mol %, (B) 0.2 mol % and (C) 0.3 mol % doping concentration of  $\text{Nd}^{3+}$  ions at room temperature

**Fig. 4** Absorption spectrum of CdS nano-material doped with (A) 0.1 mol%, (B) (A) 0.2 mol% and (C) (A) 0.3 mol% of  $\text{Nd}^{3+}$  ion



$$\alpha = 2.303 \frac{A}{t} \quad (1)$$

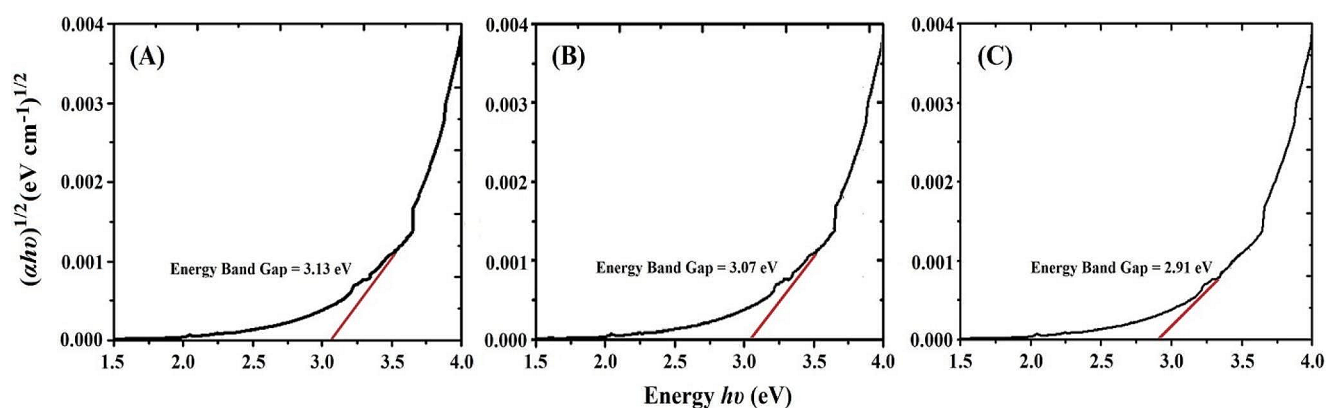
Here, the sample is taken as a solution, so the thickness is equal to the length of the 1 cm size cuvette (sample cell) size as 1 cm. The value and nature of the optical band gap energy depends on absorption coefficient. The Tauc's relation has been used to find out the value of the optical band gap using Eq. (2) [15].

$$(\alpha h\nu)^n = B(h\nu - E_g) \quad (2)$$

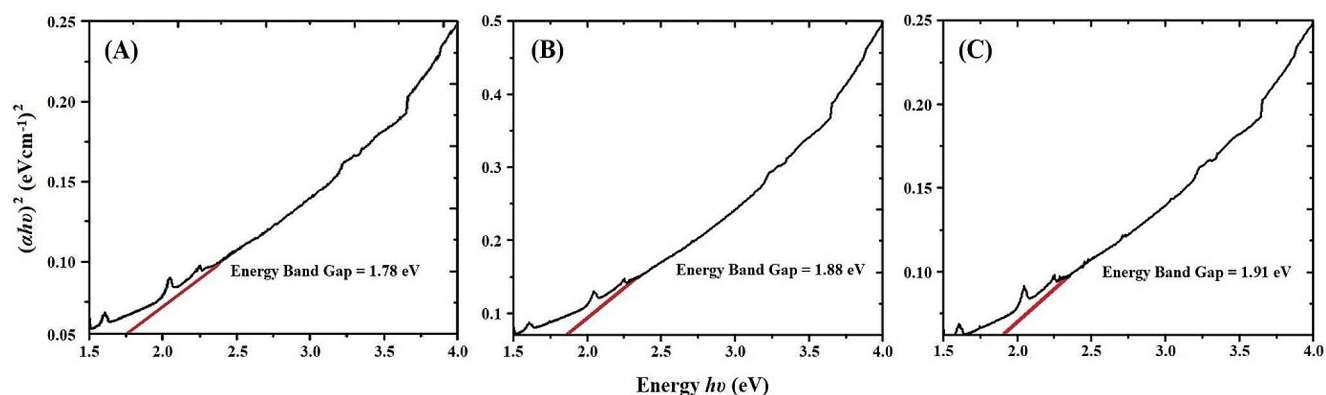
where  $h$  is Planck's constant,  $\nu$  is the frequency,  $B$  is a constant dependent on transition probability,  $E_g$  is the optical band gap energy and  $n$  is an index which indicates the light absorption process.

The value of  $n$  is 1/3, 1/2, 2/3 and 2 respectively for indirect forbidden transitions, direct allowed transitions, direct forbidden transition and indirect allowed transition [16]. In this study, the band gaps of  $\text{CdS}:\text{Nd}^{3+}$  nano-particles with different concentration (0.1, 0.2 and 0.3 mol%) of  $\text{Nd}^{3+}$  ions were calculated. Optical band gap energy and Urbach's energy are calculated from the linear part of the absorption spectra. Optical band gap is calculated by plotting a





**Fig. 5** Optical energy direct band gap of CdS: Nd<sup>3+</sup> nano-material for (A) 0.1 mol %, (B) 0.2 mol % and (C) 0.3 mol % doping concentration of Nd<sup>3+</sup> ions



**Fig. 6** Optical energy indirect band gap of CdS: Nd<sup>3+</sup> nano-material for (A) 0.1 mol %, (B) 0.2 mol % and (C) 0.3 mol % doping concentration of Nd<sup>3+</sup> ions

graph between photon energy ( $h\nu$ ) and  $(ah\nu)^{1/2}$  or  $(ah\nu)^2$  for direct transition and indirect transitions respectively. Direct band gap and indirect band gap energy values were calculated from the intersection of the extrapolated line with the photon energy axis  $(ah\nu)^{1/2} = 0$  and  $(ah\nu)^2 = 0$  respectively using the linear portion of the absorption edge of the absorption spectrum [17]. According to the calculations, the direct and indirect optical band gap for CdS:Nd<sup>3+</sup> nano-particles with different concentrations (0.1, 0.2 and 0.3 mol%) of Nd<sup>3+</sup> ions were obtained as 3.13 eV to 2.91 eV (Fig. 5) and 1.78 to 1.91 eV (Fig. 6) respectively (Table 3). As a result, the absorption edge shifted to longer wavelengths. This indicates that the direct band gap decreases with increasing concentration throughout the nano-material sample.

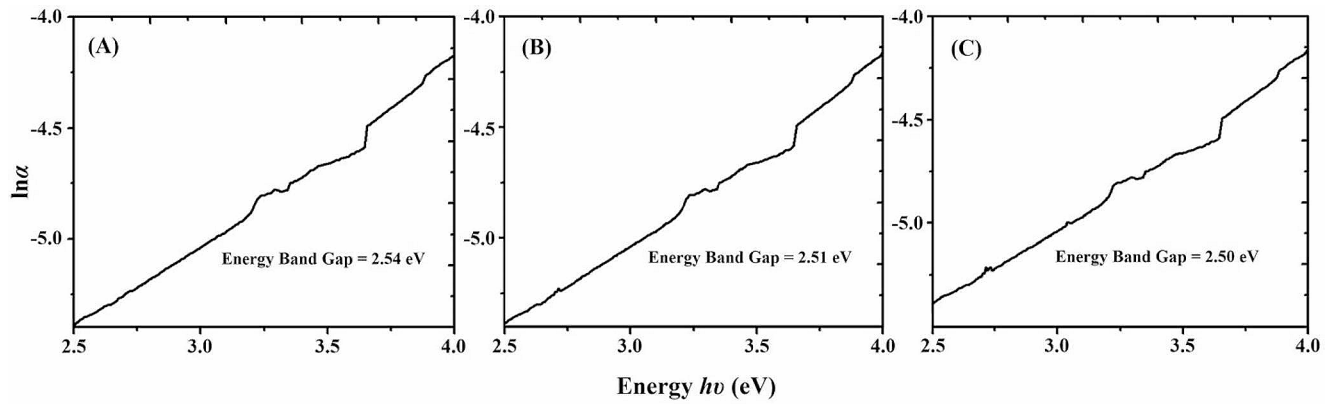
The value of  $\alpha$  at the photon energy below the optical gap depends on the photon energy [18] as:

$$\alpha = \alpha_0 e^{\frac{h\nu}{E_u}} \quad (3)$$

where  $\alpha_0$  is a constant and  $E_u$  determines the band tailing and is referred as the Urbach energy.

The Urbach's energy is obtained by plotting a graph between photon energy and  $\ln \alpha$  and extrapolating its linear part to zero and taking its reciprocal. In general Urbach's energy is almost equal to the reciprocal of optical energy band gap. The lower values of Urbach's energy indicate that prepared nanomaterials sample possess minimum defects and less disorder lines which in turn leads to structural rearrangement. Urbach energy values were calculated by taking the reciprocal of the slope of the linear part of the  $\log \alpha$  versus  $h\nu$  curve in the region lower photon energies (Fig. 7).

Urbach energy is less than the band gap energy. The Urbach energy values are between 2.54 and 2.50 eV and is shown in Table 3; Fig. 6. The Urbach energy decreases with increasing concentration of Nd<sup>3+</sup> ions. A gradual decrease in the optical band gap with precursor concentration, as observed by Urbach energy analysis can lead to an increase in grain size and a decrease in structural disorder of the materials band gap values. The synthesized nano-material can be found useful as it is suitable for its use in solar cell manufacturing, optoelectronics and radio frequency applications.



**Fig. 7** Optical Urbach energy of CdS nano-material doped with (A) 0.1 mol%, (B) 0.2 mol% and (C) 0.3 mol%  $\text{Nd}^{3+}$  ion

**Table 3** Direct and indirect energy band gap and Urbach energy of  $\text{CdS:Nd}^{3+}$  nano-particles for different concentrations of  $\text{Nd}^{3+}$  ion

$\text{Nd}^{3+}$ ion concentration	Direct band gap Energy eV	Indirect band gap Energy eV	Urbach band gap Energy eV
0.1%mol	3.13	1.78	2.54
0.2%mol	3.07	1.88	2.51
0.3%mol	2.91	1.91	2.50

**Fig. 8** Energy band (E-k) diagram for CdS nano-material doped with 0.1 mol%  $\text{Nd}^{3+}$  ions

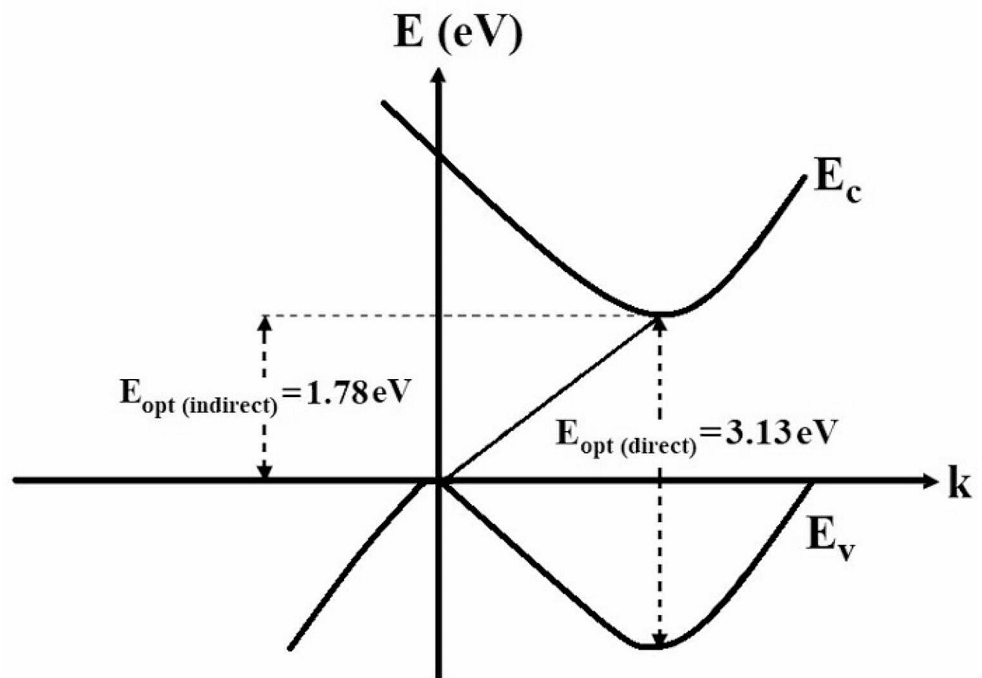


Figure 8 illustrates a schematic energy band (E-k) diagram for CdS nano-material doped with 0.1 mol%  $\text{Nd}^{3+}$  ions. In this figure we have considered direct allowed transitions for different k-space alignment of the lowest minimum of conduction band and highest maximum of valence band. From the figure it is obvious that the value of the direct band gap energy is larger than the corresponding value of the indirect band gap energy. Assuming that the existence of a conduction band minimum, there are two transitions

at the k-space and k-space maximum corresponds to direct allowed transitions and the observed indirect transitions can be related to transitions from the top the valence band to the bottom of the conduction [19].

## Conclusions

CdS:Nd<sup>3+</sup> nano-particles were synthesized by chemical precipitation method and were characterized by EDAX, XRD and absorption spectra and SEM imageries. Optical absorption spectra have been recorded in the wavelength range 400–900 nm at room temperature. From XRD analysis, particle size was determined using Debye-Scherrer formula for CdS:Nd<sup>3+</sup> nano-particles with different concentration of Nd<sup>3+</sup> ions (0.1 mol%, 0.2 mol% & 0.3 mol%). According to the result of this study, the average particle size of the CdS:Nd<sup>3+</sup> nano-particles were found to be 1–50 nm. The optical band gap energy and Urbach energy were estimated by using the absorption spectra at room temperature. The Urbach energy decreases with increase in the concentration of Nd<sup>3+</sup> ion. So, the determination of Urbach energy can directly gives a confirmation about the quantitative value of the number of defects in a semiconductor. The gradual decline in the optical band gap energy with precursor concentration may cause the increase in grain size and decrease in structural disorder in the materials as observed from Urbach energy analysis. A sharper commencement of absorption corresponds to a lower value of the Urbach energy. So, it is essentially a material parameter which can determine the shape of transition from the band tail to the mid gap states. The band gap energy values show that the synthesized nano-particle is suitable to use in solar cell fabrication, optoelectronic and high frequency applications.

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## Declarations

**Conflict of interest** The authors declare that they have NO Conflict of Interest.

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