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Research Article

OPTICAL ENERGY BAND GAP AND ABSORPTION SPECTRA OF CdS: Pr^{3+} NANOMATERIALS

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A B S T R A C T

The CdS:Pr^{3+}nanomaterial were synthesized by simple chemical precipitation synthesis method. Praseodymium ion was added in CdS:Pr^{3+} nanomaterial with different concentration 0.1, 0.2 and 0.3 mol % as a dopant. The absorption spectrum of the prepared nanomaterial have been recorded in the UV-Visible region at room temperature. The optical energy band gape of the CdS:Pr^{3+} nanomaterial were estimated through direct and indirect method from absorption spectra. The optical energy band gap decreases as the concentration of praseodymium ion increases.

INTRODUCTION

Presently, the nanoscience and technology represents the most active discipline all around the world and is considered as the fastest growing technology revolution, the human history had ever seen. This intense interest in the science of the materials confined within the atomic scales stems from the fact that these nanomaterial exhibit fundamentally unique properties with great potential of next generation technologies in electronics, computing, optics, biotechnology, medical imaging, medicine, drug delivery, structural materials, aerospace, energy etc[1-6].

One of the interesting properties of the rare-earth elements is the absorption effect produced when light is transmitted through a compound or solution in which certain of these elements are present in their trivalent state. Several members of the group show this effect in the visible region of the spectrum, and as a result when a compound or solution in which they are present is examined with the spectroscopy the absorption of certain wavelengths of the transmitted light is represented by dark line-like bands in an otherwise continuous spectrum. Doping of materials allows to noticeably modify the properties of materials.

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Because of their excellent luminescent properties, transition metal and rare earth ions doped semiconductor nanostructures have been the subject of numerous investigations[7-12].

In this paper, The CdS:Pr^{3+}nanomaterial doped with 0.1, 0.2, 0.3mol % praseodymium ion were synthesized by chemical precipitation synthesis method[13,14] and analyzed by absorption spectra. Optical energy band gap have been computed.

Experimental Details

The CdS: Pr^{3+} nanomaterial were synthesized by simple chemical precipitation synthesis method[13]. All the chemicals were of analytical grade and were used without further purification. Cadmium nitrate tetrahydrate [Cd $(NO_3)_2.4H_2O$], sodium sulphide [Na_2S], diethylene glycol [DEG], ethanol [C_2H_5OH], praseodymium chloride [$PrCl_3$] and distilled water were used as a source material. 0.1M of Cd $(NO_3)_2.4H_2O$ (50ml) was taken in conical flask. Around 20 ml of diethylene glycol (DEG) was added to cadmium Nitrate tetrahydrate solution under constant stirring. After 15 minutes, 50 ml Sodium sulphide solution and different concentration (0.1, 0.2 & 0.3 mol %) of praseodymium chloride were added drop wise under constant stirring, reaction was kept 4hrs (at 60^0C) at constant stirring and yellow precipitate of CdS formed, washed with ethanol and distill water, driedat room temperature[13,14]. The flow chart of precipitation chemical synthesis method is shown in Fig.1. The UV-Visible

absorption spectra have been recorded on 2375 Double Beam Spectrophotometer in the range 300 – 1100 nm at room temperature.

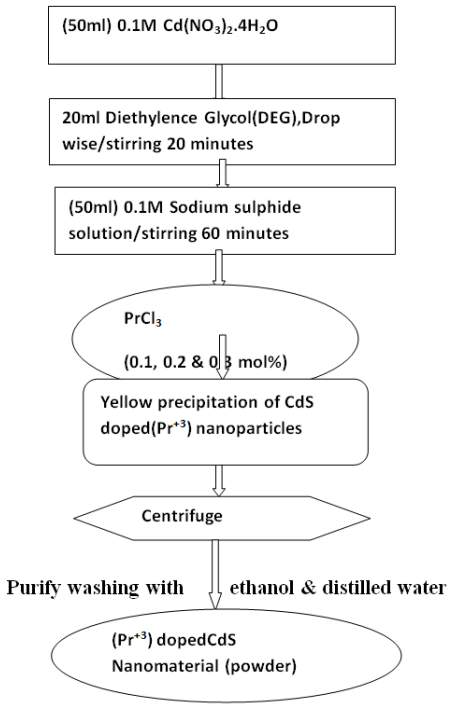

Fig 1 A flow chart Diagram of synthesis of CdS Nanomaterial with Pr^{+3}ions

RESULT AND DISCUSSION

The CdS: Pr^{3+}nanomaterial have been synthesized by chemical precipitation synthesis method with different concentration (0.1, 0.2 & 0.3 mol %) of praseodymium ion. Absorption spectra of prepared nanomaterial have been recorded in the range 300-1100nm at room temperature.

The absorption spectrum of CdS:Pr^{3+} doped with different concentration (0.1, 0.2 and 0.3 mol%) of Pr^{3+} ion sample in the range of 300-900 nm is shown in figs. 2, 3 & 4in terms of wave length between relative absorption (I_0/I), where I and I_0 are intensities of transmitted through specimens. From these curves it is noticed that absorption is dominant mainly in the blue region. This shift is due to the quantization effect according to which the band gap value increases with the size reduction of crystallites, suggesting the formation of nanometer sized CdS particles. The blue shift was observed compared with the absorption edge of the bulk CdS (Wavelength=520 nm and band gap 2.41 eV)[15,16]. The energy band gape of these materials was estimated directly and indirectly using the tauc relation[17-19].

$$E_g = h\nu/\lambda \quad (1)$$

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

where h is the Planck's constant, v the frequency, α absorbance coefficient, E_g the band gape, λ the wavelength of absorption band and n the different types of electronic transition (n=1/2 and 2 respectively for the direct and indirect transitions).

The direct and indirect optical bandgap energy was calculated using equations 1 &2. The direct optical bandgap energy values were determined from the absorption spectrum. The direct optical band gape energy values were 2.78, 2.58, 2.41, 2.15eV respectively and collected in Table 1. Similarly, the indirect energy band gape were determined from a graph (Figs.5, 6 and 7) of $(\alpha h\nu)^2$ versus hν.

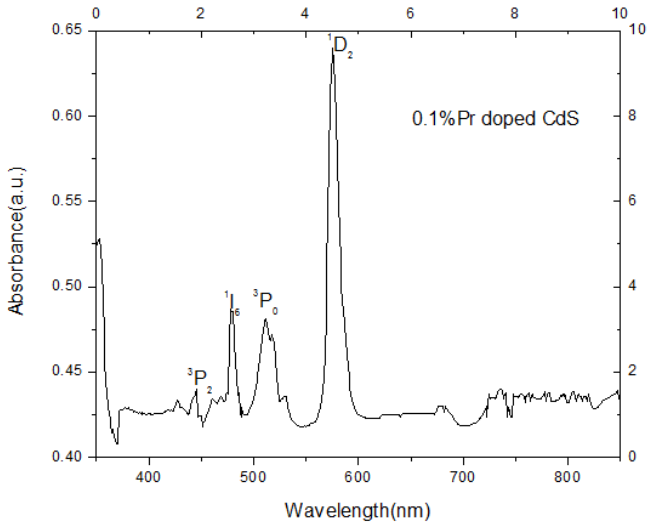

Fig 2 Absorption Spectrum of CdS Nanoparticle with Praseodymium ion (0.1 mol%)

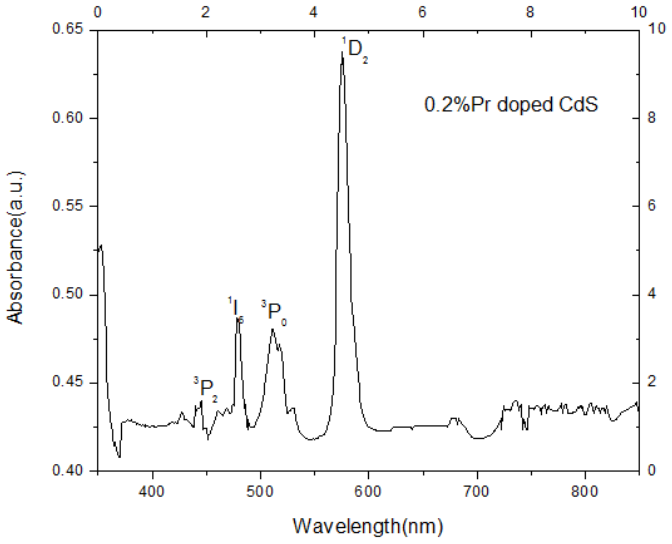

Fig 3 Absorption Spectrum of CdS Nanoparticle with Praseodymium ion (0.2 mol%)

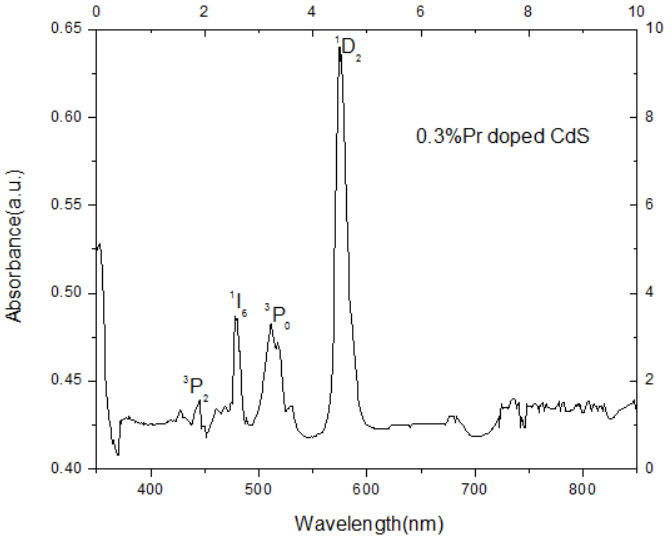

Fig 4 Absorption Spectrum of CdS Nanoparticle with Praseodymium ion (0.3 mol%)

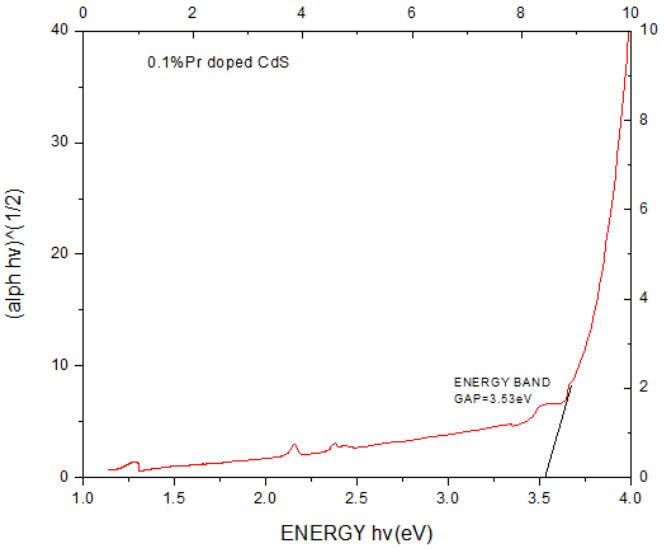

Fig 5 Optical energy band gap of CdS Nanoparticle with Praseodymium ion (0.1 mol%)

The extrapolation of straight line to $(\alpha h\nu)^2=0$ gives the value of the energy band gap of CdS:Pr^{3+} nanomaterial. From figs 5, 6 & 7, the indirect optical energy band gape for different concentration were 3.53, 3.50, 3.41 eV respectively and collected in table 2.

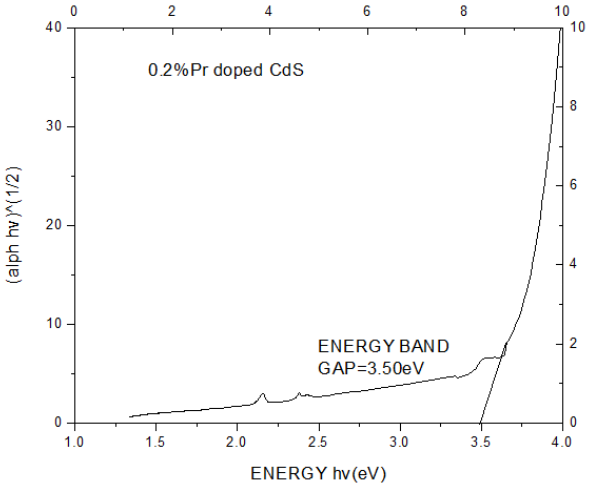

Fig 5 Optical energy band gap of CdS Nanoparticle with Praseodymium ion (0.2 mol%)

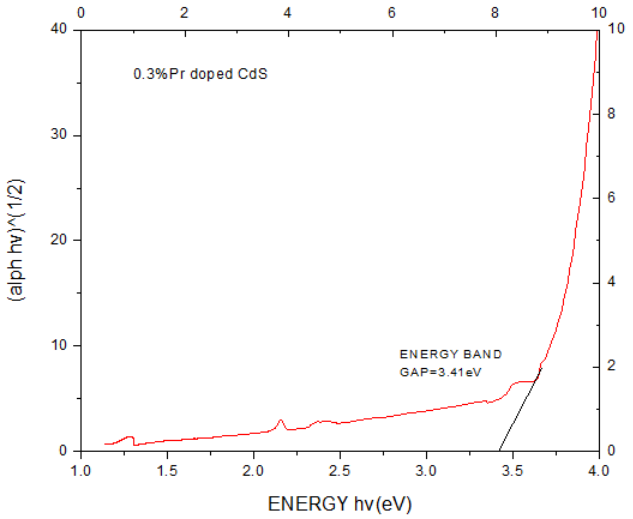

Fig 5 Optical energy band gap of CdS Nanoparticle with Praseodymium ion (0.3 mol%)

Praseodymium ion doped CdS shows a similar value of the direct optical bandgap energy, with no change in the absorption band edge of the spectrum. It reveals that incorporation of low concentration praseodymium ions does not alter the absorption properties of CdS nanocrystals. From table 2, optical energy band gap decreases as the concentration of praseodymium ion increases.

Table 1 Optical energy band gap (Eg) of CdS nanoparticle doped with different concentration of Praseodymium ion from absorption spectrum

0.1 mol %		0.2 mol %		0.3 mol %	
Wavelength λ (nm)	**Optical Energy Band gap (eV)**	**Wavelength λ (nm)**	**Optical Energy Band gap (eV)**	**Wavelength λ (nm)**	**Optical Energy Band gap (eV)**
446	2.78	445	2.78	448	2.76
480	2.58	482	2.57	481	2.57
513	2.41	512	2.42	513	2.41
576	2.15	576	2.15	577	2.14

Table 2 Optical energy band gap (Eg) of CdS nanoparticle doped with different concentration of Praseodymium ion from indirect method.

Different Concentration of Praseodymium ion	Optical Energy band gap (eV)
0.1 mol %	3.53 eV
0.2 mol %	3.50 eV
0.3 mol %	3.41 eV

CONCLUSIONS

Pr^{3+} doped CdS nanomaterial have been prepared by a simple precipitation chemical synthesis method. Optical energy band gap calculated directly and indirectly from absorption spectra. Praseodymium ion doped CdS shows a similar value of the direct optical band gap energy, with no change in the absorption band edge of the spectrum. Energy band gap decreases as the concentration of Pr^{3+} ion increases.

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