

The Influence of Capping Agents on Structural and luminescence Properties of CdS Nanoparticles

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Abstract: Cadmium sulfide nanoparticles were synthesized by using PEG, EDTA and PVP as capping agents by chemical co-precipitation technique at room temperature and as prepared samples were annealed at a temperature of 80°C. The powder X-ray diffraction (XRD) pattern revealed that CdS nanoparticles synthesized with PEG, EDTA and PVP as capping agents are in cubic phase with particle size in the range of 3-12 nm. From SEM images it was noticed that the nanoparticles with all capping agents are spherical in shape and agglomeration less in PEG capped nanoparticles. The EDAX spectrum confirms the presence of Cd and S atoms in samples with and without capping agents in near stoichiometric ratio. Photoluminescence (PL) studies revealed emission at 490 nm and 620nm. For CdS without capping agent the peak intensity is less and then increases in the order of capping agents PEG, PVP and EDTA respectively. The chemical interaction and functional groups in CdS nanoparticles were identified by FTIR spectra. Strong interactions corresponding to the CdS nanoparticles were noticed from FTIR spectra. All samples with and without capping agents exhibited diamagnetism.

Keywords: without and with capped CdS nanoparticles, Co-precipitation method, Photoluminescence, XRD, and FTIR.

1. Introduction:

The recent trends in nanoscale semiconductors have much attention because of their low dimensional dependent, chemical, physical, optical and electrical properties. Among all the semiconductors, group II-VI based semiconductors (ZnS, CdSe, ZnO, CdS etc.) plays a major role. CdS is having great potential due to narrow bandgap around ~2.4 eV at normal temperature [1-4]. CdS is very much interesting material due to its many excellent physical and chemical properties and have numerous applications in multiple technological fields. With and without capping agents of CdS possess hexagonal wurtzite structure and cubic structure [5-8]. CdS nanoparticles are having many applications, for example in flat-panel displays [9], photovoltaic cells [10], nonlinear optical devices [11], light-emitting diodes [12-14], solar cells [15, 16], photocatalysis [17], field-effect transistors [18], X-ray detectors [19], Photo detectors [20], Chemical/biological sensors [21, 22], photoconductors [23], hydrothermal treatment [24], luminescence devices [25, 8], Hydrogen production [26], etc.,

Large number of defects on the surface has non radiative pathways for excited electrons, which has high influence on the luminescent property. By adding capping agents to the surface of the material reduces the defects and dangling bond density.

CdS nanoparticles have been synthesized in various methods like hydrothermal method, chemical co-precipitation method; sol-gel method, sonochemical method and solvothermal method etc., [27-31]. Among all these methods, we have chosen a simple chemical co-precipitation method to synthesize CdS and capped CdS (PEG, EDTA, and PVP).

Herein, we report the Morphology, structural, FTIR, photoluminescence studies and magnetic studies on CdS nanoparticles with and without capping agents.

2. Experimental and characterization techniques:

2.1. Preparation of CdS nanoparticles:

Cadmium acetate dehydrate [$\text{Cd}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$] (99.5% Analytical grade) and Sodium sulphide (Na_2S) (Analytical grade), Polyethylene glycol (PEG), EDTA and Polyvinyl pyrrolidone (PVP) were used without additional purification. Deionized water is used as a solvent throughout the experiment.

CdS and Capped CdS nanoparticles were synthesized by the chemical method at room temperature. For all samples with and without capping agents the molarity was fixed at 0.2 M. Sodium sulfide solution was added drop wise to the aqueous Cadmium acetate solution, light yellow colour precipitate is formed. The final solution is magnetically stirred for 8 hours and the precipitate is washed with deionized water and ethanol for several times. The obtained precipitate was dried at 80 °C for 10 hours. In order to reduce agglomeration and to control the size of as prepared samples 2 ml of capping agents of PVP, EDTA and PEG are added to the final solution.

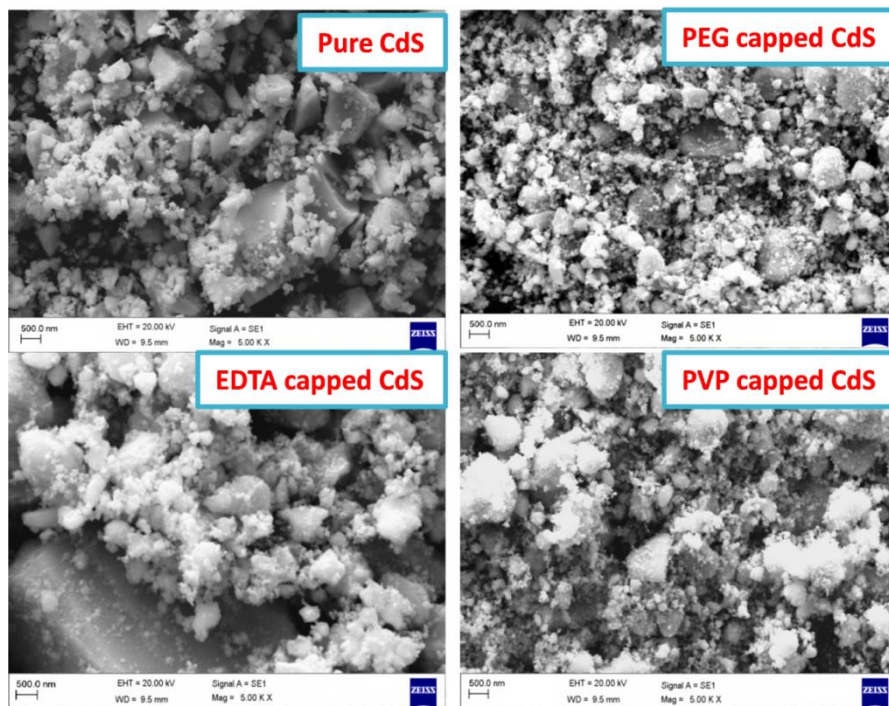
2.2. Characterization:

With and without capped CdS nanoparticles were analyzed by various characterization techniques. Surface morphology of the prepared samples was observed by scanning electron microscopy (SEM) and chemical composition by EDAX spectra. Structural properties were observed by X-ray Diffractometer with Cu-K α radiation with a wavelength of 1.5406 Å. The functional modes and elemental constituents of synthesized samples were studied by FTIR spectra. The luminescence properties were studied by photoluminescence spectra. The magnetization measurements were recorded by VSM (Vibrating sample Magnetometer) at room temperature with Lakeshore, 7410.

3. Results and discussion

3.1 Morphological studies:

The SEM images of the as prepared with and without capped CdS nanoparticles are shown in fig.1. From fig.1 it is clear that the morphology of capped CdS nanoparticles are uniform from that of the without capped CdS nanoparticles. The capped CdS nanoparticles are spherical in shape as compared without capped CdS nanoparticles. PEG capped nanoparticles are less agglomerated compared to particles with other capping agents.



.Fig.1: SEM images of with and without capped CdS nanoparticles

3.2 EDAX: Elemental Analysis:

Fig.2 shows the EDAX spectra of with and without capped CdS nanoparticles. From the figure it is clear that no other elemental peaks observed other than Cd and S in the prepared samples. This leads to the effective formation of different capped CdS nanoparticle with appreciable quality and quantity [7]. Target and estimated compositions of with and without capped CdS nanoparticles are listed in table 1.

Table-1: Compositional analysis of with and without capped CdS nanoparticles.

Sample CdS	Target composition (at %)		Estimated Composition from EDAX (at %)	
	Cd	S	Cd	S
Pure	50	50	53.50	46.50
PEG	50	50	51.76	48.24
EDTA	50	50	52.15	47.85
PVP	50	50	52.82	47.18

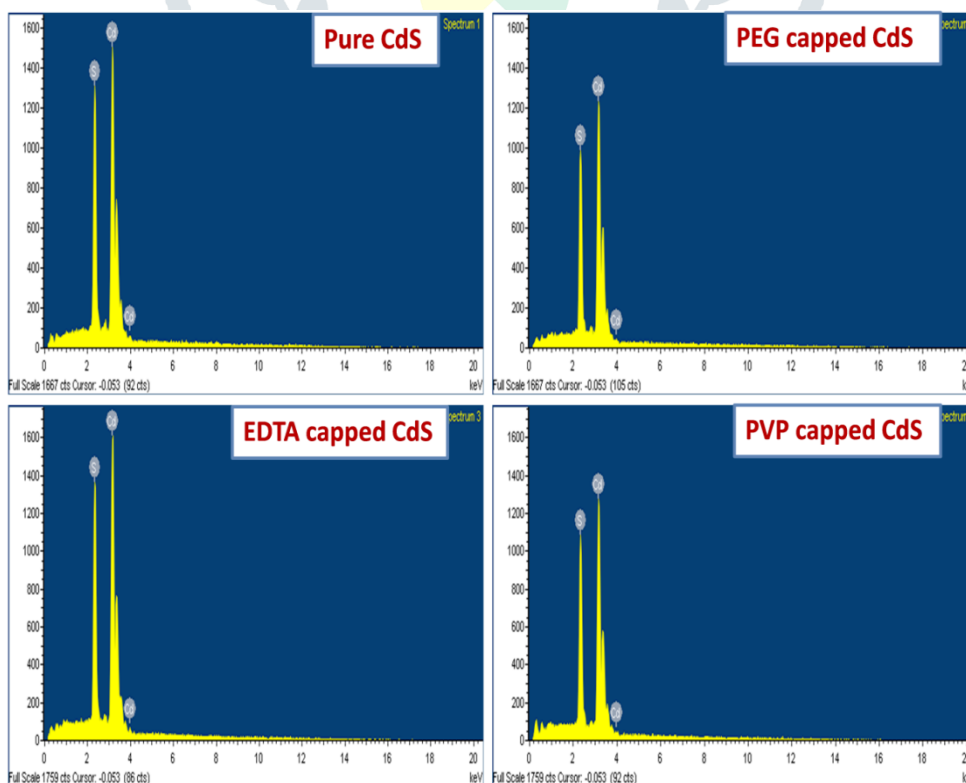


Fig.2: EDAX spectrum of with and without capped CdS nanoparticles

3.3 Structural analysis:

The influence of capping agents (PEG, EDTA and PVP) on the structural properties of CdS nanoparticles was studied by X-ray diffraction. Fig.3 shows the XRD patterns of with and without capped CdS nanoparticles maintained at constant annealed temperature of 80 °C. The XRD patterns well matched with those of the cubic CdS structure (JCPDS card No.75-1546). There is no other impurity peaks were observed in XRD patterns [8, 31]. The diffraction peaks of all samples are considerably broadened due to the decrement of particles size. The full width at half maximum (FWHM) of major peak (111) widening was used to calculate the average particle size (D) by using the Debye-Scherrer formula was in the range of 3-12 nm. The XRD parameters were tabulated in table 2.

Table-2: Structural parameters of with and without capped CdS nanoparticles

Sample CdS	d (Å) (111)	Lattice parameters a = b = c (Å)	$\alpha = \beta = \gamma$ (°)	Particle size(D) from XRD (nm)
Pure	3.285	5.78	90	12.1
PEG	3.360	5.82	90	3.0
EDTA	3.340	5.80	90	5.8
PVP	3.260	5.76	90	6.3

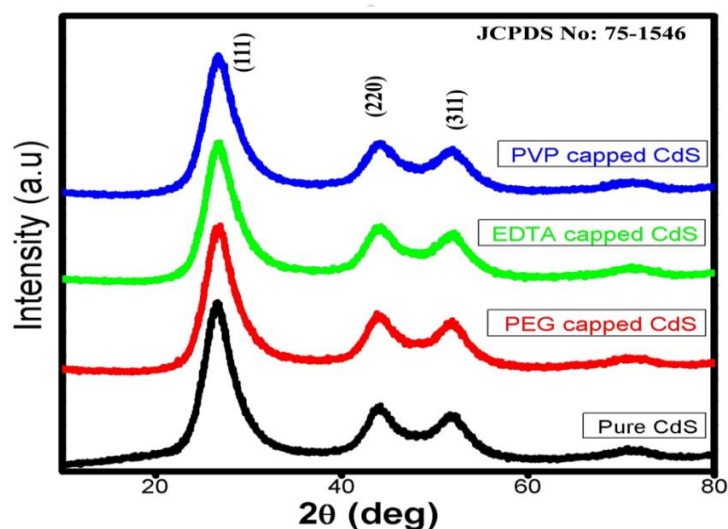


Fig.3: XRD patterns of with and without capped CdS nanoparticles

3.4 FTIR studies:

The quality of synthesized with and without capped CdS samples of FTIR studies were carried out in the range of 500 – 4000 cm^{-1} . FTIR spectra of with and without capped CdS nanoparticles are shown in fig.4. All the capped CdS nanoparticles are having the corresponding peaks have that of CdS. From fig. it is clear that the strong interactions of water molecules with CdS are reflected by the broad and strong peaks at 3420 cm^{-1} and 1622 cm^{-1} due to O-H stretching and O-H bending modes respectively [33]. The spectral band around at 3152 cm^{-1} can be assigned to capping agents and O-H groups. The bonds appearing at 2924 cm^{-1} , 1631 cm^{-1} and 1547 cm^{-1} correspond to C-H stretching and bending vibrations [28, 32].

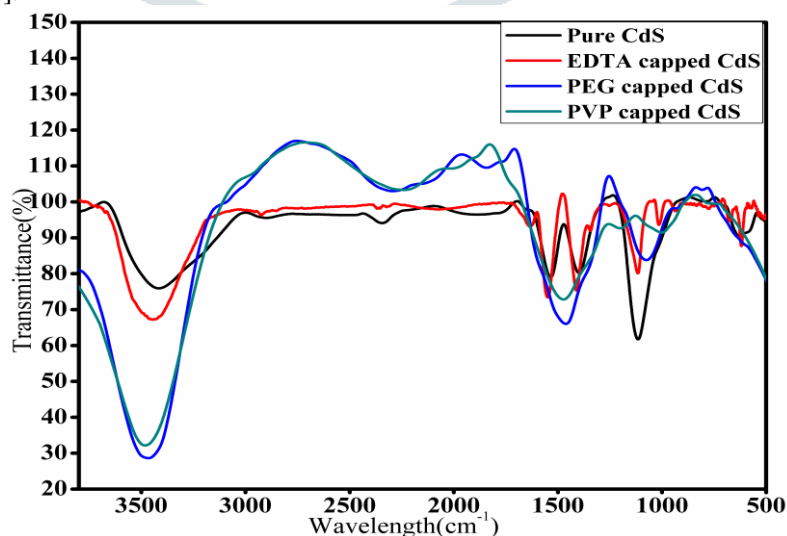


Fig.4: FTIR spectra of with and without capped CdS nanoparticles.

3.5 Photoluminescence studies:

Photoluminescence spectra give information about the defect dynamics and energies of photo generator charge carrier as well as emitting states nature. The photoluminescence response images of CdS nanoparticles at different capping agents are shown in fig.5. In the PL spectra, PEG capped CdS nanoparticles have high intensity compared to others is may be due to decrease of particle size and is attributed to increase of surface to volume ratio. At 490 nm blue emission is due to radiative recombination emission of excitation and at ~ 625 nm red emission is due to the electron transfer from conduction band to defect states in the forbidden band [7].

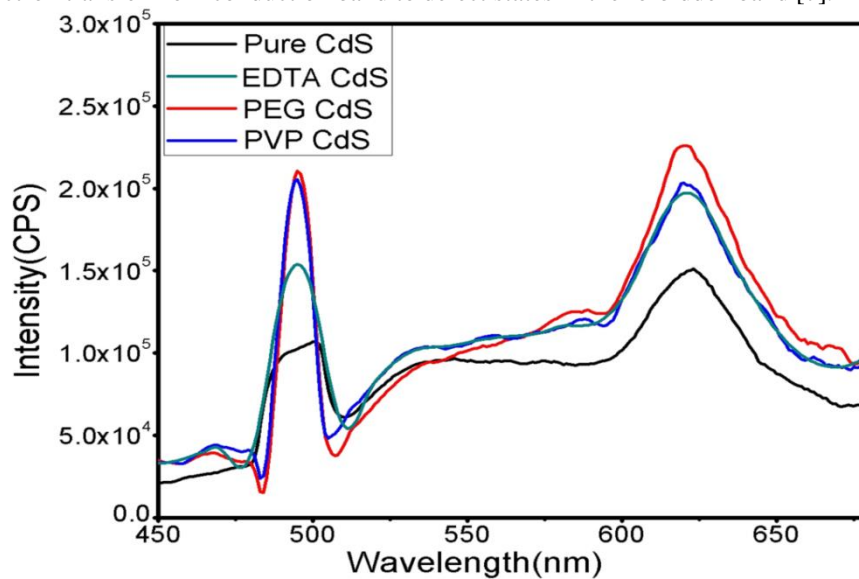


Fig.5: Photoluminescence of spectrum of with and without capped CdS nanoparticles

3.6. Magnetization studies:

Fig.6 shows the magnetization curve (M-H) for PEG capped CdS nanoparticles. The magnetization of the sample (CdS) measurements was performed at room temperature with applied magnetic field varying from -15000 to +15000 G. Due to the absence of outer unpaired electrons in Cd^{+2} and S^{-2} ions which lead to exhibit the diamagnetic nature in the samples [34, 35]. It is clear that CdS and capped CdS samples exhibit diamagnetic behaviour.

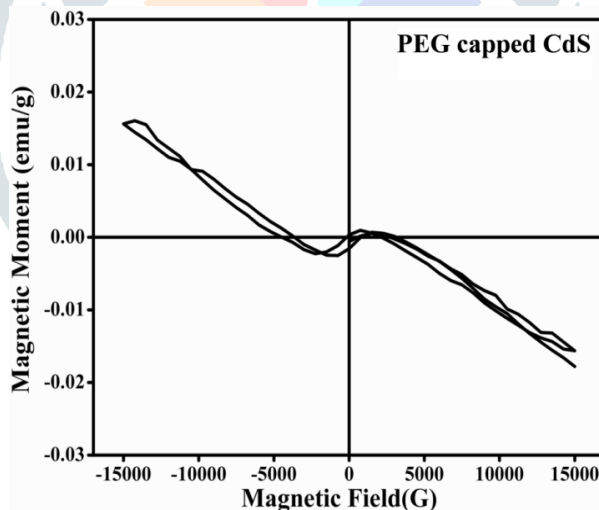


Fig. 6: Vibrating magnetometer analysis curve of PEG capped CdS nanoparticles

4. Conclusions:

In conclusion, with and without capped CdS nanoparticles were synthesized via chemical precipitation method. The XRD spectra confirmed that the structure of all prepared samples having with FCC face centered of cubic structure. The synthesized nanoparticles ranged from 3-12 nm. The SEM analysis proved that all the synthesized samples were composed spherical particles and less agglomerated with PEG capping agent. The EDAX spectra confirmed that the selective elements were observed in prepared samples. The FTIR spectra confirmed that all the chemical bonding were attributed to synthesized samples. The PL spectra confirmed a strong blue emission at ~490 nm that can be attributed to recombination of electron hole pair. All synthesized samples were exhibit diamagnetic behavior.

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