Synthesis and characterization of CdSe nanoparticles at different pH values

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Abstract:
Nanoparticles of CdSe were prepared using chemical precipitation method by varying pH value. Cadmium chloride and sodium selenide were used as precursors. CdSe NP is prepared in DETA and Sodium borohydride matrix. To vary pH values HCl is used drop by drop pH is maintained as 7.5 and 9.5. The structure of the CdSe sample is hexagonal. The crystalline size calculated by using Scherrer equation is 2.31and 2.48 nm. The UV characterization is done.

Keywords: CdSe, XRD, UV, crystalline size

1. Introduction.
In recent years much attention has been paid to the scientific and technological aspects of nanometer sized semiconductors (nano particles). These particles exhibit unique chemical and physical properties, differing substantially from those of the corresponding bulk solids. [1-2]. These differences are associated with the quantum size effect and with the existence of a relatively large percentage of atoms at the surface.

As one of the most important II-IV group semiconductors, CdSe has a direct band gap of 1.74 ev at room temperature and it is now widely used as photovoltaic device, electro luminescence and catalyst [3, 4]. High quality CdSe nanoparticles can be fabricated by several techniques such as electro deposition, evaporation [5, 6] and chemical bath deposition [7]. These methods require costly conditions. Hence simple chemical precipitation method is preferred.

CdSe nanoparticles are prepared at different pH values by chemical precipitation method. Structure and optical properties have been investigated.

2. Experimental

2.1 Materials
All chemicals were used without further purification. Cadmium Chloride (CdCl₂) and Sodium Selenide (Na₂SeO₃) were used as precursors. Double distilled water is used as solvent. Sodium Borohydride and DETA were used as ligands.

2.2 Characterization
2.2.1. XRD Analysis
The X-ray diffraction patterns for the samples were recorded using Schimadzu Labx XRD 6000 X-ray powder diffractometer with CuKα –radiations(λ=1.5406Å) for the 2θ values ranging from 10° to 90° with scanning rate 10 ° per minute.

2.2.2. Optical Characterization
The optical measurements were carried out using Varian Carry 5E spectrophotometer.

2.3. Synthesis of CdSe nanoparticles.
In the preparation of CdSe nanoparticles 0.07mol/l Cadmium Chloride solution was prepared using double distilled water. DETA solution was mixed with CdCl₂ solution. 0.07mol/l Na₂SeO₃ (100ml) solution was ordered by drop by drop with constant stirring under progressive reaction. Sodium Borohydride was added to the prepared solution. pH was adjusted for 9.5 and 7.5 by adding HCl solution. Immediately the colour changes into yellow then orange and finally into red colour.

3 Results and Discussion

3.1 XRD Analysis
XRD patterns of CdSe nanoparticles are shown in Fig1. As synthesised CdSe nanoparticles exhibited three diffraction peaks at 2θ=25.2°, 41.7° and 50.4° corresponding to the (002),(110) and (201) planes of hexagonal CdSe with the space group P63mc(186)[JCPDS NO.77-2307] with a=4.299Å and c=7.01Å. The particle size has been determined using Debye-Scherrer formula from the first peak. It is observed that the diffraction patterns of nanoparticles are broadened as pH value is increased.

Fig.1 X ray diffraction patterns of pure CdSe nanoparticles(a) sample 1 and (b) sample 2
3.2 UV
Fig 2 shows the UV/VIS optical absorption for CdSe NPs in the range 800nm to 100nm. It can be seen from the spectra that there is slight increase in observance starting from 800 to 230nm. For CdSe p\(^H\) value 7.5 sample increases in the absorption occurred at about 450 nm and peak of absorption is obtained at about 206nm. Similarly the absorption peaks for CdSe p\(^H\) value 9.5 are obtained at 204 nm. Fig 2. shows that the absorption spectra of CdSe NPs shifts toward shorter wavelengths.

Optical excitation of electron across the bandgap is strongly allowed transition, producing an abrupt increasing absorptivity at the wavelength corresponding to the gap energy. This feature in the absorption spectrum is known as the optical absorption edge. In case of nanocrystals the electronic energy levels are discretized and effective bandgap energy increases [8]. As the particle size is reduced the absorption edge shift toward blue side and absorption peak may be obtained due to discrete energy levels as in present case.

4. CONCLUSION
CdSe nanoparticles at p\(^H\) values 7.5 and 9.5 were synthesized by the chemical precipitation method employing an easy process and with better control over optical and crystalline quality. The particle size and bandgap are verified by powder XRD and UV Spectrum. X-ray diffraction patterns reveal the presence of hexagonal phase with particle size increases as p\(^H\) value increases. The optical absorption edges of the prepared CdSe samples are found to have blue shift due to high quantum confinement effect of the nanoparticles. Bandgap value of CdSe NPs increases as p\(^H\) value increased.
REFERENCES


