

# SYNTHESIS AND CHARACTERIZATION OF CTAB CAPPED CdS NANOPARTICLES

Juvin Paula A, Suresh Kumar K, Ashwini P, Bhagyalakshmi D

Aalim Mohammed Salegh College of Engineering, Avadi IAF, Chennai, India.

## Abstract:

*CTAB capped CdS nanoparticles were prepared through hydro thermal method. Structural, chemical composition and optical properties were evaluated by different analytical techniques. Powder X-ray diffraction (XRD) analysis of the CTAB capped CdS nanoparticles reveals the formation of hexagonal structure and also confirms the crystalline nature of the particles with distinct lattice environment. In Fourier transform infrared spectroscopy (FTIR), the composition of the CTAB capped CdS nanoparticles have been confirmed. Optical transition show a blue shift due to the increase of band gap energy and it is attributed to the low defects and high crystallinity. Optical band gap of pure and CTAB capped CdS nanoparticles were found to be 2.27 eV and 2.35 eV. The optical studies indicate that CdS nanoparticles with CTAB can be suitable for optoelectronic devices and photovoltaic applications.*

**Keywords:** Crystalline, CTAB, Hexagonal, Nanoparticles, Transition

## I. INTRODUCTION

Cadmium sulfide (CdS) nanocrystals have been widely investigated due to its unique properties [1,2,3]. CdS compound is a direct band gap semiconductor with its band gap of 2.4 eV for bulk hexagonal (wurtzite) structure and 2.38 eV for bulk cubic (zinc blende) structure [4]. CdS nanoparticles show attractive optical properties, upon optical excitation; the surface defect states rapidly trap the electrons and holes and quench the radiative band gap recombination [5]. CdS is now widely used for photoelectric conversion in Solar cells, light emitting diodes, photo catalysis, nonlinear optical materials, optoelectronic and biological labelling.[6]. Cetyl trimethyl ammonium bromide (CTAB) is a common cationic surfactant. Many researchers have used CTAB to fabricate a diverse variety of nanostructures like palladium nanocubes, 3D hierarchical structure of  $\text{Sr}_2\text{Sb}_2\text{O}_7$ , dendrite silver crystals, nano fibers of  $\text{BaMoO}_4$ , Copper Indium Sulphide hollow nanospheres, polyaniline nanotubules and gold nanoplates etc. Although a few works on the synthesis of CdS using CTAB have been reported [12], there are no discussions related to morphology of CdS. This motivated to explore the synthesis of CdS nanostructures using CTAB as a surfactant.

## II. EXPERIMENTAL PROCEDURE

### II. A SYNTHESIS OF CdS NANOPARTICLES

Cadmium acetate and thiourea were used as the  $\text{Cd}^{2+}$  and  $\text{S}^{2-}$  precursors respectively. NaOH was used to adjust the pH value of the solution. CTAB was used as surfactant. Acetone was used for washing purpose. 1M of cadmium acetate was dissolved in 40 ml distilled water with constant stirring. 1M of thiourea was dissolved in 40 ml and 1 g sodium hydroxide was dissolved in 20 ml distilled water. First thiourea solution was added with cadmium acetate slowly with constant stirring. Then NaOH solution was added to the original solution drop by drop to maintain a pH value of 10. The prepared final solution immediately turned yellowish orange. Then, the solution was constantly stirred for 5 hours for well mixing. Similar resembling procedure was followed for synthesis of CTAB Capped CdS nanoparticles. The only variation was, along with 0.4 g of CTAB solution was added after the thiourea solution. Finally, NaOH solution was added. Then, the slurry was transferred into a Teflon-lined stainless steel autoclave of 100 ml capacity. The autoclave was sealed and maintained at 180 °C for 12 hours and then allowed to cool to room temperature naturally. The as-formed precipitate was centrifuged, washed sequentially with deionized water and absolute ethanol and then the precipitate was dried at 70 °C for 4 hours in vacuum. Finally, the sample was annealed at 150°C for 10 hours to improve ordering.

## III. RESULTS AND DISCUSSIONS

### III. A POWDER X-RAY DIFFRACTION STUDIES

Figures 1, 2 shows the Powder X-Ray diffraction studies of the synthesized pure and CTAB capped CdS nanoparticles and it reveals the crystalline nature of the prepared samples. The average crystallite size of the as-synthesized pure and CTAB capped CdS nanoparticles were computed from the XRD pattern through the Scherrer equation [7].

$$D = k\lambda / \beta \cos\theta$$

where,  $\lambda$  is the wavelength of the Cu  $\text{K}\alpha$  X-rays (1.5405 Å),  $\beta$  is the full width at half maximum (FWHM) of the observed peak.

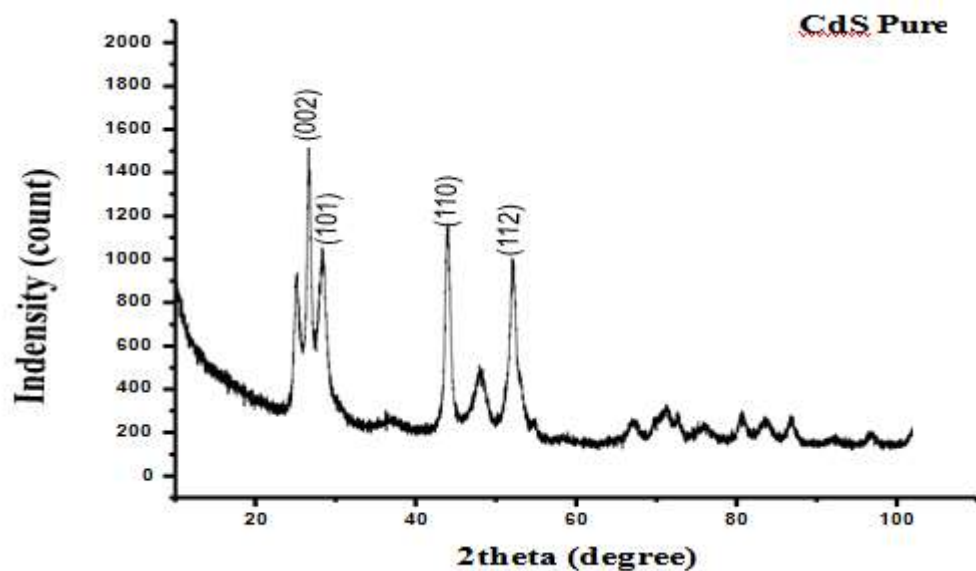


Figure:1 The XRD Pattern for pure CdS Nanoparticles

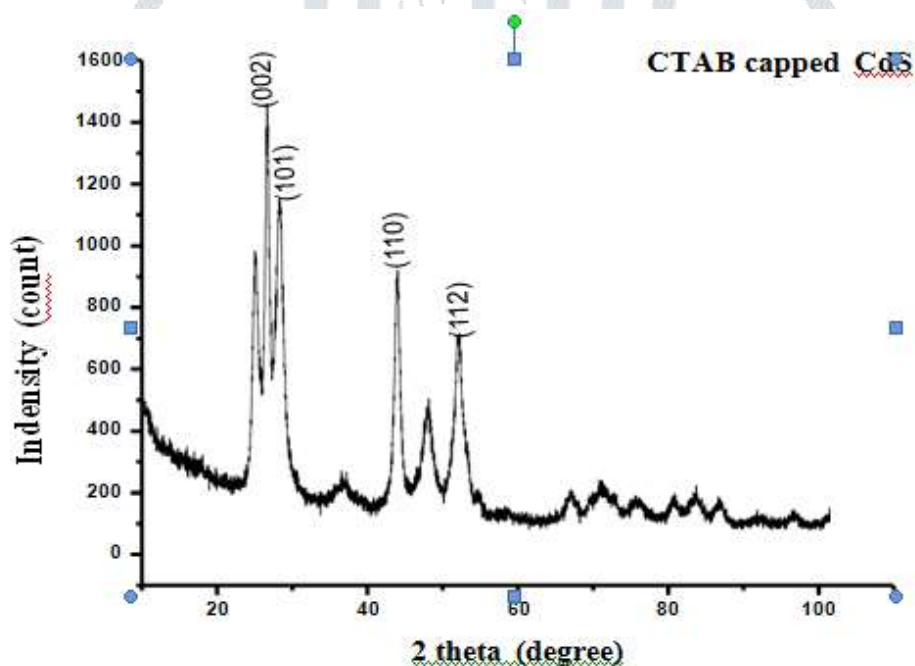


Figure: 2 The XRD Pattern for CTAB capped CdS Nanoparticles

The calculated lattice parameters are listed in Table 4.1. Diffraction peaks in the pattern could be exactly indexed to JCPDS No: 41-1049 [8]. The crystallite sizes were found to be 31 nm and 19 nm for pure and CTAB capped CdS.

Table 1: Lattice Parameters of Pure and CTAB Capped CdS Nanoparticles

|            | CdS standard<br>JCPDS: 41-1049 |           | Pure CdS<br>nanoparticles |           | CTAB capped CdS<br>nanoparticles |           |
|------------|--------------------------------|-----------|---------------------------|-----------|----------------------------------|-----------|
|            | 2 $\theta$<br>(degree)         | Intensity | 2 $\theta$<br>(degree)    | Intensity | 2 $\theta$<br>(degree)           | Intensity |
| <b>002</b> | 26.528                         | 91        | 26.6437                   | 100       | 26.5778                          | 100       |
| <b>101</b> | 28.206                         | 100       | 28.3295                   | 60        | 28.2808                          | 73        |
| <b>110</b> | 43.718                         | 48        | 43.9701                   | 78        | 43.8865                          | 60        |
| <b>112</b> | 51.869                         | 31        | 51.9257                   | 58        | 51.9613                          | 43        |
| <b>004</b> | 54.632                         | 5         | 54.6168                   | 4         | 54.7665                          | 3         |
| <b>302</b> | 86.395                         | 7         | 86.6910                   | 8         | 86.7884                          | 4         |

| Sample             | Lattice parameters |         | Volume              |
|--------------------|--------------------|---------|---------------------|
|                    | a (Å)              | c (Å)   | V (Å <sup>3</sup> ) |
| Pure CdS           | 4.22126            | 7.08805 | 109.3811            |
| CTAB<br>Capped CdS | 4.37157            | 6.58874 | 109.0457            |

### III. B FOURIER TRANSFORM INFRARED SPECTROSCOPY (FTIR) STUDIES

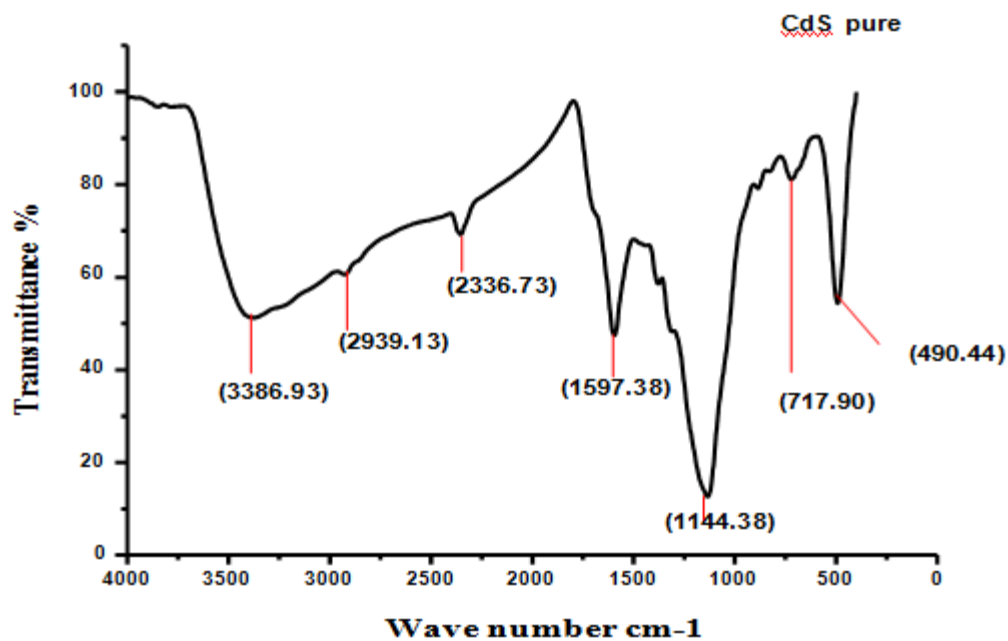


Figure 3: FTIR Spectra of pure CdS Nanoparticles

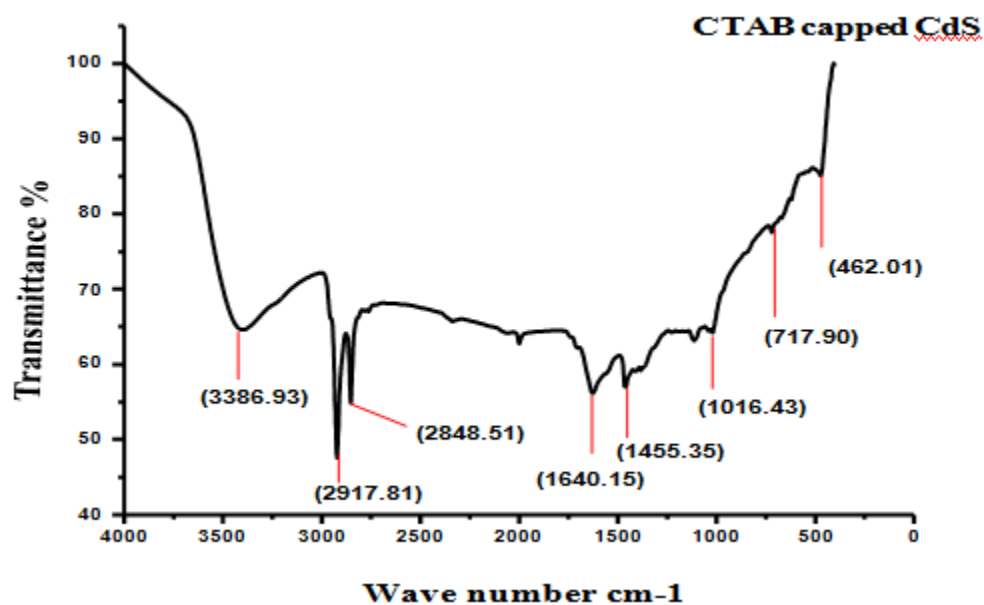


Figure 4: FTIR Spectra of pure CTAB capped Nanoparticles

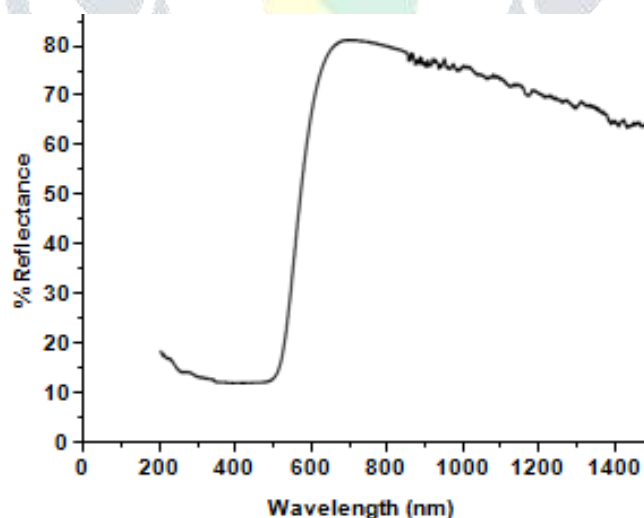
The FTIR spectrum of CdS nanoparticles were recorded in the range of 4000-500  $\text{cm}^{-1}$  and is shown in Figure 3. In the Pure CdS nanoparticles, the peak at 3386.93  $\text{cm}^{-1}$  is assigned to O-H stretching of absorbed water on the surface of CdS. The presence of water is confirmed by its bending vibration at 1597.38  $\text{cm}^{-1}$ . It is also verified by its  $\text{CH}_3$ -stretching vibrations occurring as very weak peaks just below 3000  $\text{cm}^{-1}$ . The C-O stretching vibration of absorbed methanol gives its intense peak at 1144.38

$\text{cm}^{-1}$ . There are medium to strong absorption at 610 to 723  $\text{cm}^{-1}$  possibly due to Cd-S stretching [9].

The FTIR spectra CTAB capped CdS nanoparticles are recorded in the range of 4000-500  $\text{cm}^{-1}$  and is shown in Figure 4. In the CTAB capped CdS nanoparticles, very weak absorption band is observed at 3386.93  $\text{cm}^{-1}$  is due to O-H stretching vibration of water molecules. C-C Stretching, medium strong band positions appears in the range of 1455.35  $\text{cm}^{-1}$  to 1640.15  $\text{cm}^{-1}$  and is possibly due to stretching vibrations of Sulphate group, traces of  $\text{SO}_4^{2-}$  ions. The narrow absorption peak centered at around 1016.43  $\text{cm}^{-1}$  is ascribed to the C=O bonding. There are medium to strong absorption bands at 717.90  $\text{cm}^{-1}$ , possibly due to Cd-S stretching. Hence the existences of above mentioned bands identify the presence of CdS nanoparticles [10].

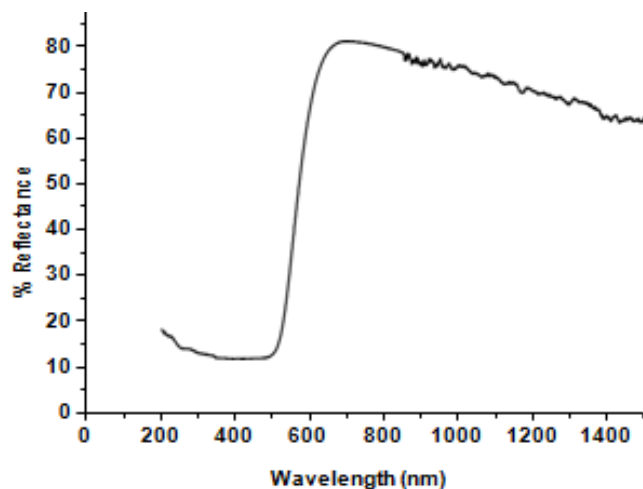
### III.C UV-vis DIFFUSED REFLECTANCE SPECTRAL ANALYSIS

The Reflectance spectra for pure and CTAB of CdS nanoparticle is shown in Figure 5 and 6. The optical band gap of pure and CTAB capped CdS were found out by extrapolating the linear portion of the energy axis at zero reflectance. The Kubelka–Munk plot is plotted between  $(\text{F(R}\infty)/\text{S})^2$  vs  $h\nu$  (eV). The Kubelka – Munk plot [9] for pure CdS and CTAB Capped CdS nanoparticles are shown in Figure 4.5 and 4.6 respectively. Hence the optical band gap of pure and CTAB capped CdS nanoparticles were found to be **2.27 eV** and **2.35 eV** respectively [11]. The optical studies indicate that CdS nanoparticles with CTAB can be suitable for optoelectronic devices and photovoltaic applications.



**Figure 5 : UV-vis Diffused Reflectance spectra of Pure CdS nanoparticles**





**Figure 6 : Reflectance spectra of CTAB capped CdS nanoparticles**

JETIR

#### IV CONCLUSION

The hydrothermal synthesis of pure and CTAB capped CdS nanoparticles has been experimentally investigated by means of XRD, UV-Vis-Spectroscopy, Photoluminescence analysis, FT-IR Analysis and TEM. The X-ray diffraction patterns show hexagonal structure for pure and CTAB capped CdS nanoparticles. The band gap energies of pure and CTAB capped CdS nanoparticles were estimated using UV-visible absorption spectra to be about 2.27 and 2.32 eV respectively. The functional groups present in the samples were confirmed by FTIR analysis.

#### References:

- [1] D. C. Harris, "Quantitative Chemical Analysis", 7th Edition, W. H. Freeman and Company, New York (2006).
- [2] A. Bollero, S. Fernandez, K. Z. Rozman, Z. Samardzija, M. Grossberg, "Preparation and Quality Assessment of CuS Thin Films Encapsulated in Glass", Thin Solid Films, 520 (2012) 4184.
- [3] K. D. Yuan, J. J. Wu, M. L. Lui, L. L. Zhang, F. F. Xu, L.D. Chen, F. Q. Huang, "A Fabrication and Microstructure of P-type Transparent Conducting CuS Thin Film and its Application in Dye-Sensitized Solar Cell", Applied Physics Letter, 93 (2008) 132-106.

- [4] Y. Chen, C. Davoisne, J. M. Tarascon, C. Guery, "Influence of Thickness on the Photosensing Properties of Chemically Synthesized Copper Sulfide" *Thin Films Chemistry*, 22 (2012) 5295.
- [5] S. Y. Kuchmii, A. V. Korzhak, A. E. Raevskaya, A. I. Kryukov, "Quantum Size Effects in Semiconductor Photocatalysis", *Theoretical and Experimental Chemistry*, 37 (2001) 31.
- [6] W. Qingqing, Z Gaoling, H Gaorong, "Properties of Polymer Nanocomposites on the Basis of Heterostructures Ag<sub>2</sub>S/CdS", *Material Letters*, 2005, 59, 2625-2629.
- [7] Zhang Jun, Di Xiao-Wei, Liu Zhi-Liang, Xu Gang, Xu Sheng-Ming, Zhou Xing-Ping, "Multicolored Luminescent CdS nanocrystals", *Transactions of Nonferrous Metals Society of China* 17 (2007) 1367.
- [8] G.Q. Xu, B. Liu, S.J. Xu, C.H. Chew, S.J. Chua, L.M. Gana, "Luminescence Studies of CdS Spherical Particles Via Hydrothermal Synthesis", *Journal of Physics and Chemistry of Solids*, 61 (2000) 829–836.
- [9] J. Joo, H.B. Na, T. Yu, J.H. Yu, Y.W. Kim, F. Wu, J.Z. Zhang, T. Hyeon, "A Generalized and Facile Synthesis of Semiconducting Metal Sulfide Nanocrystals", *Journal of the American Chemical Society*, 125 (2003) 11100–11105.
- [10] B. Srinivasa Rao, B. Rajesh Kumar, V. Rajagopal Reddy, T. Subba Rao, "Preparation and Characterization Of CdS Nanoparticles By Chemical Co-Precipitation Technique", *Chalcogenide Letters*, Vol. 8, No. 3, March 2011, P. 177 – 185.
- [11] Saravanan L, Diwakar S, Mohankumar R, Pandurangan A, Jayavel R, "Structural Properties of CdS Nanoparticles for Solar Cell Applications", *International Journal of Pure and Applied Sciences and Technology*, 23(1) (2014), pp. 8-12.
- [12] Yi Ding, Guangtao Zhang, Hao Wu, Bin Hai, Liangbin Wang, and Yitai Qian, "Nanoscale Magnesium Hydroxide and Magnesium Oxide Powders: Control Over Size, Shape, and Structure Via Hydrothermal Synthesis", *Chemistry of Materials*. 2001, 13, 435-440.