**ABSTRACT**

Cadmium sulphide (CdS) and zinc sulphide (ZnS) are important group II-VI semiconductor material with many excellent physical and chemical properties which has many applications in multiple technical fields including photochemical catalysis, gas sensor detectors for laser and infra red solar cells, non-linear optical materials, various luminescence devices and optoelectronic devices etc. CdS and ZnS nanoparticles doped with $Mn^{2+}$ are successfully synthesized by chemical co-precipitation method using polyvinyl alcohol (PVA) as capping agent. The advantages of using chemical co-precipitation method are that the method is not only simple and economical but also has the capability to produce size controlled nanoparticles. PVA is used as capping agent especially during synthesis because it controls particle agglomeration and passivate the semiconductor surface against surface defect. This capping agent molecule binds to the surface of the particle by stabilizing the nuclei and prevents agglomeration hence controlling the growth of nanoparticle. The influence of various $Mn^{2+}$ concentrations on the structural, morphological and optical properties of nanoparticles have been investigated and discussed. Doping with $Mn^{2+}$ ion provides good traps for the excited electrons which give rise to their potential use in non-linear optics, electronic and optoelectronic devices. The prepared nanoparticles are crushed into powder and then characterized.

Structural characterization of the synthesized samples has been performed using X-ray diffraction (XRD). XRD patterns show that the dopant atoms of $Mn^{2+}$ are incorporated at the Cd and Zn sites in cubic structure without disturbing original CdS and ZnS cubic zinc blende structure. Transmission electron microscope (TEM) also confirms that the particles are in the range of 3.95 nm - 5 nm for CdS:Mn and in the range of 3.45 nm - 4.85 nm for ZnS:Mn. HRTEM images clearly show the lattice fringes which indicates the crystalline nature of the synthesized samples and Selected area electron diffraction (SAED) pattern observed from TEM show the cubic zinc blende structure

which are in consistent with XRD pattern. Scanning electron microscope (SEM) and Energy dispersive X-ray (EDX) analysis have been used to study the morphology and elemental analysis of the synthesized samples. EDX spectra confirm the presence of manganese ($Mn^{2+}$) in the samples with expected stoichiometry. Absorption study have been carried out by using UV-vis spectrophotometer to determine the band gap of CdS:Mn and ZnS:Mn nanoparticles. Radius of the synthesized nanoparticles has been evaluated from the absorption spectrum by using Effective mass approximation (EMA) formula. The effect of $Mn^{2+}$ substitution on the photoluminescence properties of undoped and doped samples has also been studied. The presence of the capping agent has been revealed by Fourier transform infrared spectra (FTIR).

The thesis is organised into seven chapters and brief discussions are given below.

Chapter 1 gives the general introduction of nanotechnology and nanomaterials. The chapter discusses the origin of nano followed by a brief discussion on different types of nanomaterials. It also explains the various properties and application areas of nanomaterials. CdS and ZnS compound are also briefly reviewed in this chapter.

Chapter 2 presents the scenario of earlier research works on doped and undoped CdS and ZnS nanoparticles with and without capping agent and their results.

Chapter 3 describes the various synthesis approaches for the preparation semiconductor nanomaterials followed by different methods for preparing nanomaterials. The importance and use of chemical co-precipitation method has also been stated along with the role of capping agent and polyvinyl alcohol during the synthesis process.

Chapter 4 gives a brief description of different characterization techniques. The chapter includes the theoretical and experimental work that is involved in the characterization of nanoparticles like X-ray diffraction (XRD), Transmission electron microscope (TEM), Scanning electron microscope (SEM), Energy dispersive X-ray

(EDX) analysis, UV-vis spectroscopy, photoluminescence (PL) spectra and Fourier transform infrared (FTIR) spectroscopy etc.

Chapter 5 describes the details about the synthesis and characterization of PVA capped CdS nanoparticles doped with different concentration of $Mn^{2+}$. The chapter contains the structural analysis by XRD, TEM, HRTEM and SAED; morphological and compositional analysis by SEM and EDX and optical analysis by UV-vis spectroscopy, photoluminescence and FTIR spectroscopy. From the XRD results, the crystal structure with identification of phase, lattice constant, dislocation density, average strain along with crystallite size obtained using Debye Scherrer formula are determined. The spherical shape of the synthesized nanoparticles is confirmed from the TEM images. Characterization by SEM provides microscopic information of the surface structure and roughness. Optical properties have been used to determine the band gap of the synthesized samples. Radius of the synthesized samples has been determined using EMA formula which agrees well with XRD data. In this chapter, luminescence properties of the sample have been described and presence of the capping agent has also been confirmed from FTIR spectra.

Chapter 6 explains the synthesis and characterization of PVA capped ZnS nanoparticles doped with different concentration of $Mn^{2+}$ and its structural, morphological, compositional and optical characterization by XRD, TEM, HRTEM, SAED, SEM, EDX, UV-vis spectroscopy, photoluminescence and FTIR spectroscopy. The crystal structure with identification of phase, lattice constant, dislocation density, average strain along with crystallite size obtained using Debye Scherrer formula are determined from the XRD results. The spherical shape of the synthesized nanoparticles is confirmed from the TEM images. Characterization by SEM provides microscopic information of the surface structure and roughness. Optical properties have been used to determine the band gap of the synthesized samples. Like in the case of CdS:Mn nanoparticles, the radius of the synthesized samples is also determined using EMA formula which agrees well with XRD data. In this chapter, luminescence properties of the

sample have also been discussed which illustrates that $Mn^{2+}$ doping not only enhance the optical transition efficiency but also exhibit interesting optical properties of ZnS nanoparticles. The presence of the capping agent has also been confirmed from FTIR spectra.

Chapter 7 gives a short summary of the thesis as well as avenues for future work.