

## **Band gap of cubic and hexagonal CdS quantum dots - experimental and theoretical studies**

### **ABSTRACT**

CdS quantum dots of face centered cubic (fcc) and hexagonal close packed (hcp) structures were synthesized from sulphur source of sodium sulphide and thioacetamide respectively via microwave-hydrothermal method. The synthesized quantum dots were characterized using X-ray diffraction (XRD), transmission electron microscopy (TEM) and UV-visible spectrophotometry. The average particle size in the range 8.5 - 12.5 nm increases with the increase of microwave exposure time from 10 to 40 min. Particles with hcp structure are larger than those with the fcc structure. The band gap in the range 2.54 - 2.65 eV decreases with the increase of microwave exposure time and the particles with the hcp structure have larger band gap than those with the fcc structure. The band gap of the CdS quantum dots were also derived from time independent Schrodinger equations for CdS system and calculated using the density functional theory (DFT). There is good agreement between the measured and calculated band gap values. The results also reveal that the band gap decreases with the increase of particle size due to the quantum size effects.

**Keyword:** Band gap; CdS quantum dots; Crystal structures; DFT; Optical absorption; Particle size