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Thesis Title: "**Study of Spectroscopic and Optoelectronic properties of Semiconductor Clusters and their Semi-empirical and ab-initio Computations**"

Thin films and nanoparticles of II-VI group semiconductor materials have been investigated by material scientists due to their excellent optical, structural, electrical, magnetic, dielectric, piezoelectric and optoelectronics properties. CdS, CdTe and ZnO are the important members of II-VI group. These materials play key role in micro electronics, optoelectronics, solar cell and various industrial applications. The present investigations are focused on the experimental and theoretical studies of semiconductor thin films and nanoparticles of CdS, CdTe and ZnO whose thin films have been fabricated by thermal evaporation and sol-gel technique on silicon and glass substrates. The CdS nanoparticles have been synthesized by the chemical displacement reaction using cadmium nitrate as the cadmium source and sodium sulfide as a sulfur source. The characterization of the samples is done using the XRD, SEM, UV-VIS, FTIR, Raman spectroscopy, photoconductivity, electrical conductivity and dielectric measurements. On theoretical side, the density of states and band structures of synthesized materials are calculated and are compared with the experimentally determined values. The major outcomes of the present work are outlined below:

- CdS thin films clusters have been fabricated on the Si (100) wafers and glass substrate by the thermal evaporation technique. The band gap of the thin films on Si (100) and glass substrate

is found to be 2.50 eV and 2.42 eV respectively. It is found that the structural, optical and electrical properties are similar on both the substrate and very little difference is observed in various properties. So CdS thin films on Si (100) substrate have similar behavior as on glass substrate, indicating the fabrication of good quality CdS thin films on Si (100) substrate useful for applications.

- CdS thin films are deposited on the glass substrate of different thickness by thermal evaporation technique. The CdS thin films are found to be polycrystalline in nature. On increasing the thickness, the crystallinity of the thin films is found to be improving whereas the band gap of thin films is found to increase. The thin films with thickness around the 500 nm, shows the bulk properties of CdS materials.
- Synthesis of CdS nanoparticles using the chemical displacement reaction has been carried out. An enhancement in the dielectric properties of synthesized CdS nanoparticles accompanied by a blue shifting in the band edge has been observed.
- Undoped and Cd doped ZnO thin film on quartz substrate are fabricated using the sol-gel spin coating method. The band gap and transmission of the undoped ZnO thin films are observed to be 3.30 eV and 90-92% in the range of visible region of solar cell spectrum respectively. A red shift in band edge and a decrease in percentage transmission are observed in ZnO due to the Cd-doping.
- On theoretical side, ab-initio computations for the calculation of DOS, band gap and band structure are carried out for CdS hexagonal wurtzite structure, cubic zinc blende structure of CdS nanoparticles, CdTe cubic zincblende and hexagonal wurtzite ZnO. Semi-empirical calculations using PM3 method are also carried out to study the effect of Cd-doping in ZnO on the value of band gap.