

Abstract Submitted  
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**Excitonic effects in optical absorption spectrum of CdS/ZnSe core-shell Nanostructures.** KALUM PALANDAGE, GAYANATH FERNANDO, RAMPI RAMPRASAD, University of Connecticut, JAMES DAVENPORT, Brookhaven National Lab — We have used a first principles, TDDFT method to study CdS (Type I) nanocrystal quantum dots and CdS/ZnSe core/shell (Type II) heteronanostructures with high accuracy. We have studied the existence of excitons and multi-excitons and the possibility of optical gain in these nanoclusters. The size dependence of the HOMO-LUMO gap, electron-hole wave function overlap in the relevant states, coordination of atoms at the surface as well as the stability of such clusters will be presented in some detail.

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