Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Investigation of the effect of core/shell interface on exciton binding energy and electron-hole recombination probability in CdSe/ZnS quantum dots JENNIFER ELWARD, ARINDAM CHAKRABORTY, Department of Chemistry, Syracuse University — The explicitly correlated configuration interaction (XCCI) method is a variational technique in which an explicitly correlated reference wavefunction is used for performing the CI calculations. This work presents a multi-faceted study of the effect of heterojunction in nanoparticles and detailed analysis of various influential factors. The XCCI method was used for the study and the calculations were performed in three stages. In stage 1, the CdSe core was kept at a fixed size and the ZnS shell thickness was increased. In stage 2, the dot size was kept fixed and volume ratio between the core and the shell was varied. In stage 3, the sharpness of the core/shell interface was investigated by performing calculations on a core/alloy/shell system. Exciton binding energy (EB) and electron-hole recombination probability (eh-RP) were computed and the results were compared with CdSe quantum dots with similar radii. The presence of the heterojunction was found to effect the scaling of EB and eh-RP as a function of dot size. It was also found that EB and eh-RP scale very differently with respect to dot sizes. Expectation value of r_{eh} and radial 2-particle eh-reduced density matrix were used for analysis of spatial distribution of the quasiparticles in the multilayered qdots.

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Date submitted: 16 Nov 2012 Electronic form version 1.4