Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Calculation of exciton binding energy and electron-hole recombination probability in quantum dots using explicitly correlated electron-hole wavefunction based method ARINDAM CHAKRABORTY, Syracuse University — Accurate description of electron-hole correlation plays a central role in describing optical properties of quantum dots. This talk will focus on development of explicitly correlated wavefunction based methods for accurate treatment of electron-hole correlation. In this method, the wavefunction depends explicitly on the electron-hole inter-particle distance (R12) term and electron-hole wavefunction is obtained using variational procedure by minimizing the total energy. In inclusion of R12 term allows for a better description of wavefunction at small electron-hole distances and is found to be crucial for calculation of accurate electron-hole recombination probability and binding energy. The 2-particle electron-hole reduced density matrix (2-RDM) is obtained from the optimized wavefunction and the electron-hole recombination probability is computed from the diagonal elements of the 2-RDM. The developed method is applied to InGaAs/GaAs, CdSe/ZnS, and InP/InGaP quantum dots and exciton binding energy and electron-hole recombination probability are computed for a range of dot sizes. The computed results are compared with experimental results and path-integral Monte Carlo and configuration interaction calculations.

Arindam Chakraborty
Syracuse University

Date submitted: 29 Nov 2011 Electronic form version 1.4