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**Investigation of electron-hole recombination in multi-layered quantum dots using explicitly correlated wavefunction based methods** ARINDAM CHAKRABORTY, Syracuse University — Electron-hole pairs are generated by photoexcitation of electrons to excited electronic states. Accurate calculations of electron-hole binding energies and recombination probabilities can give important insights into the photovoltaic properties of semiconductor nanocrystals and quantum dots. In the present work, the challenge of accurate treatment of electron-hole correlation is addressed by developing explicitly correlated electron-hole wavefunction that depends on electron-hole interparticle distance. The explicitly correlated ansatz for the electron-hole wavefunction is used to calculate eigenvalues and eigenfunction of the electron-hole Hamiltonian in multi-layered quantum dots using self-consistent field (SCF) and configuration interaction (CI) techniques. These methods are applied to investigate influence of the core/shell structure and chemical composition on electron-hole binding energies and recombination probabilities. The calculations indicate that for a given chemical composition there exists a optimum core/shell structure than minimizes electron-hole recombination. Comparison with experimental studies on similar system show good agreement between the experimental and computed results.

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