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Development of accurate electron-hole exchange-correlation functional for calculation of exciton binding energy and electron-hole recombination probability in quantum dots ARINDAM CHAKRABORTY, CHRISTOPHER BLANTON, Syracuse University — Development of electron-hole exchange-correlation functional (eh-Exc) is challenging because of various factors such as distance dependent dielectric function, different effective masses, and presence of core/shell interfaces. Calculation of eh-recombination probability is also challenging because of its sensitivity to the form of the wavefunction at small electron-hole separation. This talk will focus on systematic development of eh-Exc to address these challenges. In this approach an orbital based functional is constructed by combining the strategy of direct minimization of the optimized effective potential (OEP) with the OEP-MBPT method. The eh-Exc functional was used for computational of exciton binding energy and eh-recombination in a series of CdSe qdots. Comparison of the eh-Exc results with pseudopotential+CI calculations, Kohn-Sham perturbation theory calculations, and experimental values will be presented. The results indicate that the search for the ground state densities can be restricted to a set of N-representable densities which satisfy the electron-hole Kato cusp condition. Assessment and benchmarking of the quality of the eh-recombination probability will be presented by comparing eh-Exc results with explicitly correlated methods such as PIMC and QMC calculations.

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