

Development of electron-hole correlation functional for investigation of optical properties of quantum dots

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Electron-hole pairs in quantum dots are generated by photoexcitation of electrons to excited electronic states. For application of quantum dots as efficient light-harvesting materials, it is important to have a reduced probability of electron-hole recombination. In this work, the electron-hole correlation in quantum dots is investigated using electron-hole density functional theory. The electron-hole correlation functional plays a central role in determining the accuracy of the calculations. In the present work, explicitly correlated electron-hole wavefunction is used as a starting point to generate reduced density matrices and the 2-particle electron-hole reduced density matrix is used to develop electron-hole correlation functional. A novel feature of this strategy is that the developed functional is not only used for calculation of energy but is also used for calculation of the electron-hole recombination probability. The quality of the developed functional is assessed by performing calculation on benchmark systems and comparing the results from explicitly correlated wavefunction based methods and full configuration interaction (FCI) calculations.