

Abstract Submitted
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Describing electronic excitations using electron-hole density functional theory (eh-DFT) ARINDAM CHAKRABORTY, Syracuse University — The electron-hole interaction play a crucial role in calculating optical properties of atoms, molecules, clusters and solids. In this talk, the density functional treatment of electron-hole quasiparticle interaction will be presented in the framework of electron-hole density functional theory(eh-DFT). The electron-hole correlation functional plays a central role in accuracy of any eh-DFT calculations. In the present work, the development of eh-correlation functional using the eh-reduced density matrix will be presented. Benchmark calculation using the developed functional will be compared with HF, full CI, R12-full CI, and explicitly correlated Hartree-Fock calculations. Exciton binding energies in CdSe quantum dots have been calculated and the eh-DFT results will be compared with experimental and pseudopotential+CI results. Discussion on construction of electron-hole adiabatic connection curve (ACC) using density-constrained minimization will be presented and the results from the ACC will be compared with eh-DFT calculations. Finally, similarity and difference between the GW+Bethe-Salpeter method and eh-DFT approach for treating electron-hole interaction will be presented.

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