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A Combined TDLDA/GW/CI Methodology for Multi-Exciton Processes[1] MARK LUSK, ZHIBIN LIN, Colorado School of Mines, ALBERTO FRANCESCHETTI, National Renewable Energy Laboratory, RENEWABLE ENERGY MATERIALS RESEARCH SCIENCE AND ENGINEERING CENTER COLLABORATION — A computational methodology is introduced to facilitate the analysis of multi-exciton processes in photo-voltaic systems. Time-domain density functional theory within the local density approximation (TDLDA) is used to estimate the dynamic polarization response of molecules and small quantum dots. The response function is then used to estimate screening in a real-space implementation of screened Green function (GW) theory that is employed to construct quasi-particle wave functions. A linear combination of singly- or doubly-excited Slater determinants is constructed from these states and subjected to a variational argument in order to obtain the weighting coefficients. Significantly, a screened Coulomb interaction based on the TDLDA polarization response is used in the associated Hamiltonian. The methodology is used to quantify the rate of impact ionization, as compared with competing relaxation processes, in small CdSe quantum dots.

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