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Auger Relaxation of Hot Electrons in CdSe Quantum Dots using GFSH DHARA TRIVEDI, Department of Physics & Astronomy, University of Rochester, LINJUN WANG, OLEG PREZHDO, Department of Chemistry, University of Southern California — We carry out *ab initio* nonadiabatic molecular dynamics (NAMD) simulations to study the fast relaxations of hot electrons in a CdSe quantum dot (QD). The reviewed system is a promising candidate for QD-sensitized semiconductor solar cells and the presence of well-separated conduction electron states opens the possibility of energy selectivity for hot carriers. We examine the intraband relaxation of the photoexcited electrons in the QD and the role of surface ligand in the process. A novel global flux surface hopping (GFSH) approach is adopted. We investigate the electron relaxation from the 1Pe to 1Se state in pure and 1,6-hexanedithiol ligated CdSe QD. The intraband relaxation is accelerated due to the Auger-type relaxation in the pure QD. The ligand forms a hole trapping state, which competes with the Auger-type relaxation impeding the electron-hole energy exchange. The present study establishes the basic theoretical model describing the relaxation processes in both scenarios. The model is supported by computational studies of relaxation dynamics in model QD-ligand complexes. The obtained interplay between the competing phonon-assisted Auger and ligand-induced trapping mechanisms has given us a comprehensive picture of the complex photoinduced dynamic related to QDs.

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