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Dynamical processes in semiconductor nanoclusters PENG HAN, GABRIEL BESTER, Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — We study the electronic relaxation processes via electron-phonon interaction in colloidal semiconductor nanoclusters (NCs) using the Liouville-von Neumann equation including a phenomenological Lindblad decay term. The electron-phonon coupling matrix elements used in our study are obtained from frozen-phonon calculations based on *ab initio* density functional theory (DFT). To estimate the phonon lifetime of NCs, which is used in the Lindblad decay term, we perform *ab initio* molecular dynamics simulations of a $Si_{10}H_{16}$ cluster and extract the time evolution of the energy of selected vibrational modes from the energy auto-correlation functions. We find vibrational cooling times of around 0.1 ps for high frequency Si-H vibrations, and cooling time of around 1 ps for pure Si modes, which are close to the phonon lifetimes in bulk Si. Analyzing the electronic relaxation processes with the parameters from DFT calculations, we observe a decaying Rabi oscillation with a period of tens of femtoseconds corresponding to the emission/absorption of a phonon. We notice that the Rabi oscillation frequency is proportional to the electron-phonon coupling strength while the decay process is dominated by the phonon lifetime and the energy detuning.

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