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Applications of the Reduced-Density-Matrix Description to Electronic Relaxations in Solids and Nanostructures Due to Scattering by Phonons[1] ALEX KUTANA, Rice University, VERNE JACOBS, Naval Research Laboratory — We show some examples of the application of our reduced-density-matrix description to electronic relaxations in solids and nanostructures. We carry out first-principles calculations for the relaxations of excited electrons due to scattering by phonons, using density functional theory (DFT), ab initio electronic structure methods, and reduced-density-matrix theory (RDMT) in the isolated-line and short-memory-time (Markov) approximations. Our description allows calculating properties related to the dynamical behavior of electrons in these systems without using any of the customary approximations. The main ingredients in these calculations – electronic energy levels, dipole-transition matrix elements, and analytical electron-phonon coupling matrix elements – are obtained entirely from first principles. In this work, we apply the theory to study the behavior of electrons and holes in the bulk phase as well as at the interface between two nanoscale materials. We evaluate carrier lifetimes and quantify charge and energy transfer in these systems. We also calculate line widths and shifts that are then used to construct theoretical linear absorption spectra, which are compared with experimental results.

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