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Ab Initio Calculations for Electronic Relaxations in Molecules and Solids Due to Scattering by Phonons[1] ALEX KUTANA, VERNE JACOBS, Naval Research Laboratory, CENTER FOR COMPUTATIONAL MATERIALS SCIENCE TEAM — We carry out first-principles calculations for relaxations of excited electrons in molecules and solids due to scattering by phonons. Density matrix theory (DMT) is employed, which allows for a rigorous evaluation of electronic lifetimes, line widths and shifts, entirely from first principles. The three main ingredients in these calculations – electronic energy levels, dipole-transition matrix elements, and electron-phonon coupling matrix elements – are obtained from configuration interaction (CI) and density functional theory (DFT). Combining DMT, CI, and DFT allows one to avoid the use of the empirical line widths, as commonly employed in most previous investigations, and instead calculate their values from first principles. The calculated line widths and shifts are used to construct theoretical linear absorption spectra, which are then compared with experimental results.

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