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Time-dependent density functional approach for ultrafast optical phenomena[1] VOLODYMYR TURKOWSKI, CARSTEN A. ULLRICH, Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211 — We present a formulation of time-dependent density functional theory (TDDFT) in a density-matrix framework, which can be applied to study ultrafast optical phenomena in semiconductor bulk systems and heterostructures. In particular, we derive and analyze the TDDFT version of the semiconductor Bloch equations and study the resulting absorption spectra of simple model insulators for different types of exchange-correlation potentials within and beyond the adiabatic LDA. We discuss the demands that the time-dependent exchange-correlation potential needs to satisfy in order to obtain physically correct absorption spectra, including excitonic features.

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