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Time-dependent density-functional approach for exciton binding energies¹ VOLODYMYR TURKOWSKI, CARSTEN A. ULLRICH, Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211 — We use TDDFT to study ultrafast electron dynamics and excitonic effects in insulators and semiconductors. Within a two-band approximation of the linearized semiconductor Bloch equations, we derive a TDDFT version of the Wannier equation for excitonic wave functions and binding energies. The TDDFT Wannier equation produces in principle the exact excitonic spectrum. However, this puts stringent requirements on the exchange-correlation (XC) kernel. We analyze various XC kernels that lead to bound excitonic states, and propose new model XC kernels designed to reproduce experimental exciton spectra.

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