Abstract Submitted
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Time-dependent density-functional approach for exciton binding energies[1] ARITZ LEONARDO, Department of Physics and Astronomy, University of Missouri, Columbia, Missouri 65211, USA, VOLODYMYR TURKOWSKI, Department of Physics and NanoScience Technology Center, University of Central Florida, Orlando, Florida 32816, USA, CARSTEN A. ULLRICH , Department of Physics and Astronomy, University of Missouri, Columbia, Missouri 65211, USA — Optical processes in insulators and semiconductors, including excitonic effects, can be described using time-dependent density-functional theory (TDDFT) in linear response, provided one uses suitable long-range exchange-correlation (XC) kernels. We derive a conceptually and computationally simple formalism for calculating exciton binding energies with TDDFT which is convenient for testing different XC kernels. The formalism is based on a linearization of the TDDFT semiconductor Bloch equations within a two-band model and gives rise to an eigenvalue equation in momentum space which directly yields exciton binding energies; these can be accurate even if the underlying Kohn-Sham band gap is not. Exciton binding energies are calculated for several direct-gap semiconductors and insulators using exchange-only and model XC kernels.

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