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A minimal TDDFT model for excitons¹ YONGHUI LI, ZENGHUI YANG, CARSTEN ULLRICH, University of Missouri — Optical processes in insulators and semiconductors, including excitonic effects, can be accurately described with linear-response TDDFT, provided one uses suitable exchange-correlation kernels. We have developed a conceptually and computationally simple formalism for calculating exciton binding energies with TDDFT, based on a two-band approximation. This formalism is implemented in a one-dimensional Kronig-Penney model, and we discuss the requirements for excitonic binding in this model. The performance of different types of exchange-correlation kernels (long- versus short-ranged, adiabatic versus nonadiabatic) is analyzed, with a particular emphasis on the excitonic Rydberg series.

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Yonghui Li University of Missouri

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