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Excitons in solids with time-dependent density-functional theory: the long-range corrected kernel and beyond YOUNG-MOO BYUN, CARSTEN ULLRICH, Univ of Missouri - Columbia — Time-dependent density-functional theory (TDDFT) can describe the optical properties of solids in principle more efficiently than the Bethe-Salpeter equation, but the construction of good approximations to the exchange-correlation (xc) kernel is challenging. Since the long-range ($-1/q^2$) behavior is a key for producing bound excitons in solids, many long-range corrected (LRC) xc kernels have been proposed, among them the so-called "bootstrap" kernel. However, closely related LRC-type kernels have been reported in the literature to yield conflicting results. Here, we reveal the origin of the confusion, present a new choice-free LRC kernel which yields exciton binding energies of semiconductors and insulators accurately and efficiently, and discuss the general limitations of LRC-type xc kernels. This work was supported by NSF Grant DMR-1408904

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