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Direct calculation of exciton binding energies with time-dependent density-functional theory[1] ZENGHUI YANG, CARSTEN ULLRICH, University of Missouri - Columbia — Excitons are coupled electron-hole pairs below the band gap in bulk semiconductors. They are vital to photovoltaics, but they are hard to obtain in a TDDFT calculation, due to usually employed exchange-correlation kernels lacking the long-range part. Another difficulty comes from the usual method of applying TDDFT on bulk materials which calculate the spectrum - though suitable for continuum excitations, this approach does not upfront yield the binding energy of the discrete excitonic excitations. We develop a method in analog with the Casida equation formalism, in which exciton binding energies are obtained directly. We calculate exciton binding energies for both small- and large-gap semiconductors with this method. We study the recently published "bootstrap" exchange-kernel within our method, and we extend the formalism to treat triplet excitons.

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