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Excitons in time-dependent density-functional theory[1]

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Excitons are the dominant feature in the optical spectra of insulators and semiconductors close to the absorption edge. They are collective excitations of the many-body system, but can often be discussed in a simplified picture as bound electron-hole pairs. To describe excitons in bulk materials with time-dependent density-functional theory (TDDFT), exchange-correlation functionals with a proper long-range behavior are required. The first part of this talk will present a TDDFT approach for directly calculating singlet and triplet exciton binding energies, which is based on an adaptation of the Casida formalism for periodic solids. Several exchange-correlation kernels have been tested for a variety of semiconductors and large-gap insulators. The second part of this talk will discuss a method to visualize exciton dynamics in large organic molecules in real time, based on the time-dependent transition density matrix. The method is applied to study the optical properties of intramolecular charge-transfer excitons in photoexcited molecular donor-acceptor systems that are of interest in organic photovoltaics.

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