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Long-range excitations in time-dependent density functional theory DAVID G. TEMPEL, NEEPA T. MAITRA, Hunter College of CUNY — Within TDDFT linear response, an adiabatic approximation such as ALDA to the exchange correlation kernel is most often used. It is local in time, or when considered in the frequency domain, frequency independent. We show that this neglected frequency dependence leads to drastic consequences for all excitations of a heteroatomic molecule composed of two open shell fragments at large separation. Strong frequency dependence of the kernel is needed for excitations of both local and charge transfer character. The needed frequency dependence arises from static correlation due to the step in the Kohn Sham potential between the fragments. An approximate kernel is derived to undo the static correlation and restore excited molecular dissociation curves at large separation. Leading order polarization and local dynamic correlation effects are also included. Future challenges for TDDFT will be discussed including molecular Feshabch resonances in stretched systems.

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