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Long Range Charge-Transfer Excitations in Time-Dependent Density Functional Theory NEEPA MAITRA, Hunter College of the City University of New York — Long-range charge-transfer excited states are notoriously badly underestimated in time-dependent density-functional theory (TDDFT). Yet charge-transfer is an important and ubiquitous phenomena in, for example, biological molecules, which are large enough that TDDFT appears the only practical approach. In this talk, I discuss how charge-transfer excitations between open-shell species is accurately recovered in *exact* TDDFT: in particular, the role of the step in the ground-state potential, and the severe frequency-dependence of the exchange-correlation kernel.

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