

Abstract Submitted
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Discontinuities of the exchange-correlation kernel and charge-transfer excitations in time-dependent density functional theory MARIA HELLGREN, Max-Planck-Institute, Weinberg 2, Halle(Saale), Germany, E.K.U. GROSS, Max-Planck-Institute, Weinberg 2, Halle (Saale), Germany — We identify the key property that the exchange-correlation (XC) kernel of time-dependent density functional theory (TDDFT) must have in order to describe long-range charge-transfer excitations. We show that the discontinuity of the XC potential as a function of particle number induces a frequency-dependent discontinuity of the XC kernel which diverges in the dissociation limit. This divergency compensates for the exponentially small overlap between the acceptor and donor orbitals, thereby yielding a finite correction to the Kohn-Sham eigenvalue differences. This mechanism is illustrated to first order in the Coulomb interaction.

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