Long-range corrected TDDFT and its applications

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Long-range corrected (LC) TDDFT [1] has been applied to various subjects in TDDFT calculations. As a result, the underestimations of long-range charge transfers and Rydberg excitation energies and oscillator strengths have already been solved by LC-TDDFT [1]. We implemented LC-TDDFT on the analytical gradient algorithm of TDDFT [2]. At first, we applied it to various geometry optimizations of excited states. By calculating several adiabatic excitations, it was found that LC-TDDFT makes it possible to estimate accurate excitation energies and excited state geometries especially for charge transfer excitations. Especially, we succeeded to make clear the whole twisted intramolecular charge transfer (TICT) mechanism of 4-N,N-dimethylaminobenzonitrile (DMABN) [3]. We recently applied this LC-TDDFT gradient algorithm to anharmonic vibrational state calculations [4].

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