

Recent progress in long-range corrected density functional theory

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Recent studies on long-range corrected (LC) density functional theory (DFT) [1] and its applications are presented.

So far, it has been reported that LC-DFT solves or clearly improves various properties that conventional DFTs have seriously failed to reproduce: e.g. van der Waals and other weak bond energies and structures [2], optical properties of long-chain molecules [3] and diradicals [4], and charge transfer energies and oscillator strengths in time-dependent DFT (TDDFT) [5]. In particular, it was recently found that LC-DFT quantitatively reproduces valence orbital energies for the first time [6]. We have recently suggested that several properties are unexpectedly poorly reproduced are clearly improved by using LC-DFT. In this talk, I will introduce these properties and will explain why these are significantly improved by LC-DFT.

However, there remains several serious problems that cannot be solved even by LC-DFT. We have worked on finding out these problems and have suggested new approaches to solve them. For example, we found that long-range correction hardly affects core excitation energies in TDDFT that have been significantly underestimated in TDDFT even using up-to-date functionals. To improve these core excitation energies, we have therefore suggested a regional self-interaction correction method, in which short-range exchange functionals in the regions of self-interacted electrons are only replaced with Hartree-Fock exchange integral based on the pseudo-spectral method. We have also made it possible to calculate spin-orbit splittings of excitation energies in TDDFT by implementing spin-orbit couplings into TDDFT program. I will briefly review these correction methods for LC-DFT in this talk.

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