Joint CQSE and CASTS Seminar

Weekly Seminar
Dec. 7, 2012 (Friday)

TIME Dec. 7, 14:30 ~ 15:30
TITLE Development and Benchmark of New Multi-Coefficient Double-Hybrid Density Functional Theory with SCS-MP2 and MP4 Corrections
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Abstract

We have developed a series of Multi-Coefficient Density Functional Theory (MC-DFT) that effectively extrapolates the basis set to optimal sizes. Significant improvement on thermochemical kinetics prediction was obtained for various hybrid and double-hybrid density functionals (HDFT and DHDFT) usually with high computational efficiency. The performance of MC-DFT can be further improved combining energies from *ab initio* MP2 and SCS-MP2 calculation with one or more basis sets. The method MC-DSD-BLYP | MC-SCS-MP2 with the basis set combination of [pdz/ptz/apdz] gives an mean unsigned errors (MUE) of only 0.92 kcal/mol, well within chemical accuracy, on 109 atomic energies, 13 ionization potentials, 13 electron affinities, and 76 reaction barrier heights at reasonable computational cost and with affordable size scaling. Adding energy components from MP4 calculation with suitable basis set combination can further reduce the MUE to 0.73 kcal/mol with moderate increase in computational costs. The MC-DFT|MC-SCS-MP2 and MC-DFT|MC-MP4 methodologies were proved to be economical alternatives to high-level *ab initio* or large-basis-set DFT calculation to predict reliable energies for thermodynamics and kinetics study.