Long-range correction using the Yukawa potential in density functional theory

Yoshinobu Akinaga, Seiichiro Ten-no

Graduate School of Information Science, Nagoya University, Chikusa-ku, Nagoya 464-8601, Japan
CREST, Japan Science and Technology Agency (JST), 4-1-8 Honcho Kawaguchi, Saitama 332-0012, Japan

Abstract

The long-range correction (LRC) in density functional theory (DFT) has drawn extensive interest in recent years [1]. The electron-electron interaction is separated into short-range (SR) and long-range (LR) parts using a suitable range-separation function. While the exchange interaction arising from the SR component is expressed by a density functional, the LR interaction is treated in the form of Hartree-Fock (HF) exchange energy. The complementary error function erfc(μr) has been adopted for the range-separation function for the ease of the computation of two-electron integrals over the modified Coulomb operator with Gaussian-type basis functions. Recently we have implemented and tested [2] new LRC schemes where the Slater function exp($-\gamma r$) is adopted for the range-separation function instead of erfc(μr). The resulting SR component of the Coulomb operator, the Yukawa potential, is expected to be physically more sound choice for the SR potential. A method developed in explicitly correlated F12 theory using Slater-type geminals allows us to compute two-electron integrals over the Yukawa potential with Gaussian basis functions [3]. Our benchmark results clearly show that the use of the Yukawa potential instead of erfc delivers improvements in reproducing both atomization energies and excitation energies.

---

[1] A. Savin and H. –J. Flad, *Int. J. Quantum Chem.*, **56** (1995) 327.

[2] Y. Akinaga and S. Ten-no, *Chem. Phys. Lett.*, **462** (2008) 348; *Int. J. Quantum Chem*., in press.

[3] S. Ten-no, *Chem. Phys. Lett.*, **398** (2004) 56; *J. Chem. Phys.*, **126** (2007) 014108.