P−06

短距離と長距離を補正した密度汎関数法(LCgau-DFT)の開発

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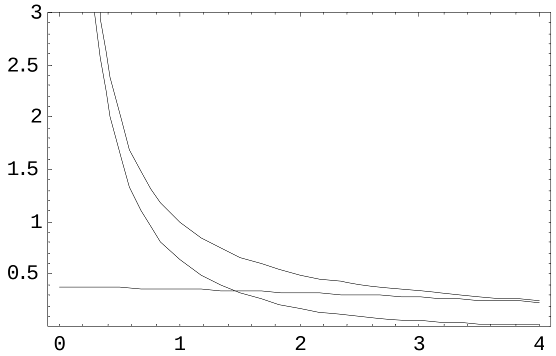
In the LC scheme, the exchange functional is partitioned with respect to the inter-electronic separation into long-range and short-range parts using a standard error function like



$$E_{DFT}[\rho] = T_s[\rho]+E_{ne}[\rho]+J[\rho]+\underline{E_x[\rho]}+E_c[\rho]$$

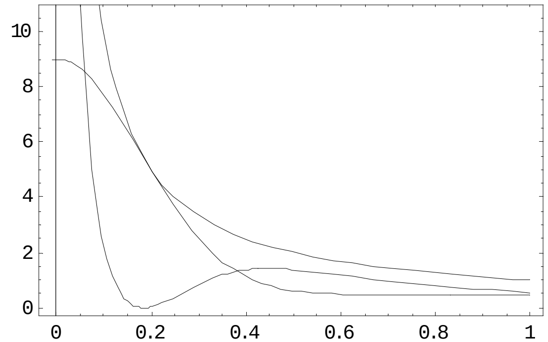
$$\frac{1}{r_{12}} = \frac{\mathrm{erf}(\mu r_{12})}{r_{12}} + \frac{1-\mathrm{erf}(\mu r_{12})}{r_{12}}$$

HF DFT

LCgau-DFT includes the modification in exchange functional partitioning with a Gaussian function with two parameter, *a* and *k*.

$$\frac{1}{r_{12}} = \frac{\mathrm{erf}(\mu r_{12})}{r} - k\frac{2\mu}{\sqrt{\pi}}e^{-(1/a)\mu^2 r^2} + \frac{1-\mathrm{erf}(\mu r_{12})}{r} + k\frac{2\mu}{\sqrt{\pi}}e^{-(1/a)\mu^2 r^2}$$

HF DFT



- A new hybrid exchange-correlation functional based on the LC scheme, named LCgau-DFT, is demonstrated to be consistently superior to other such functionals, including LC-BOP, CAM-BLYP, and B3LYP, in terms of the reproduction of atomization energies, barrier heights, reaction enthalpies, geometrical properties, and excitation energies (including charge-transfer excitations) over a wide range of molecular systems.