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

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

\[ \frac{1}{r_{12}} = \frac{\text{erf}(\mu r_{12})}{r_{12}} + \frac{1 - \text{erf}(\mu r_{12})}{r_{12}} \]

HF DFT

LCgau-DFT includes the modification in exchange functional partitioning with a Gaussian function with two parameters, \( a \) and \( k \).

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

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.