

X-PBE:

J.P. Perdew, K. Burke and M. Ernzerhof, “Generalized gradient approximation made simple”, *Phys. Rev. Lett.*, 77(18):3865–3868, 1996

$$K = \sum_s pbex,$$

where

$$kp = 0.804,$$

$$\mu = 0.2195149727645171,$$

$$\begin{aligned} kF &= n \\ &\mapsto \sqrt[3]{3} \sqrt[3]{\pi^2 n}, \end{aligned}$$

$$\begin{aligned} eX &= n \\ &\mapsto -3/4 \frac{kF(n)}{\pi}, \end{aligned}$$

$$\begin{aligned} FX &= s \\ &\mapsto 1 + kp - kp \left(1 + \frac{\mu s^2}{kp} \right)^{-1}, \end{aligned}$$

$$\begin{aligned} S &= (n, s) \\ &\mapsto 1/2 \frac{\sqrt{s}}{kF(n) n} \end{aligned}$$

and

$$pbex = \rho_s eX (2 \rho_s) FX (S (2 \rho_s, 4 \sigma_{ss})).$$

To avoid singularities in the limit $\rho_s \rightarrow 0$

$$G = pbex.$$

Bibliography

J.P. Perdew, K. Burke and M. Ernzerhof, “Generalized gradient approximation made simple”, *Phys. Rev. Lett.*, 77(18):3865–3868, 1996.