Density scaling in non-interacting kinetic energy functional development

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The influence of enforcing an approximate density scaling condition[1] in a non-interacting kinetic energy functional is investigated. A generalised gradient approximation (GGA) is presented and its performance is assessed for the computation of non-interacting kinetic energies and diatomic potential energy curves. Results are compared with other local/GGA functionals from the literature.

1. A. Borgoo, A. M. Teale, and D. J. Tozer, J. Chem. Phys. **136** 034101 (2012)