Laplacian-based models for the exchange energy. [1]

ANTONIO C. CANCIO, CHRISTOPHER E. WAGNER[2], SHAUN WOOD, Ball State University — Recent Quantum Monte Carlo data for the exchange-correlation energy density of pseudopotential systems strongly suggest the value of using the Laplacian of the density as a variable for constructing first order corrections to the local density approximation of density functional theory. We report on an exchange functional built upon these observations and extended to the all-electron case. The model keeps the typical properties of constraint-based generalized gradient approximations (GGA) and also has a finite-valued potential at the nucleus, unlike the GGA. Problems with oscillatory behavior in the potential due to higher order derivatives are controlled by a curvature minimization constraint. The results are tested against exact potentials for the He and Ne atom. A combination of gradient and Laplacian as suggested by a gradient expansion of the exchange hole gives the best overall results.

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