

# Construction of a New Meta-Generalized Gradient Approximation

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## Abstract

Meta-generalized gradient approximations (MGGAs) make use not only of the local electron density and its gradient (as in GGA's), but also the kinetic energy density and /or the Laplacian of the electron density. While the correlation part of the PKZB MGGA [1] is satisfactory, its exchange part is empirically fitted to atomization energies of molecules and produces bond lengths for molecules that are less accurate than those of GGA. Here we construct a new MGGA for exchange as an interpolation between functionals designed for the weakly-inhomogeneous and strongly-inhomogeneous limits. For the weakly inhomogeneous limit, we start from the second-order gradient expansion of the exchange hole around an electron, then make a real-space cutoff of its spurious long-range part. This is the same procedure used to construct the Perdew-Wang 1991 GGA, with one important difference: We do not make an integration by parts to convert second derivatives of the density into first derivatives. In the slowly-varying limit, the resulting functional naturally recovers the fourth-order gradient expansion of the exchange energy. For the strongly-inhomogeneous limit, we use a functional constructed from the density matrix expansion.

[1] J. P. Perdew, S. Kurth, A. Zupan, and P. Blaha, *Phys. Rev. Lett.* **82**, 2544 (1999).

