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Beyond the LDA in density functional theory: empirical Laplacian-based models for the exchange-correlation energy. ANTONIO C. CANCIO, Ball State University, M.Y. CHOU, Georgia Tech — We report recent work in developing a simple GGA-level density functional theory using primarily the Laplacian of the density $\nabla^2 n$ as an input beyond the LDA, obtained by a fit to the exchange-correlation energy density of the Si crystal and atom¹. Preliminary tests of this model with LDA pseudopotentials for several solids and molecules show a modestly improved treatment of structural properties over that of conventional GGA's, particularly for covalently bonded systems. We discuss an all-electron generalization of our model constructed by fitting to all-electron data for the energy density and potential of closed-shell first row atoms (He, Be, Ne)². The use of $\nabla^2 n$ trivially avoids the singularity in the Kohn-Sham potential that gradient-based models suffer due to the cusp in electron density at the nucleus. Using an expansion in $1/\nabla^2 n$ we are able to fit exchange energy densities in the cusp region with a great degree of accuracy, while obtaining reasonable potentials.

¹A. C. Cancio and M. Y. Chou, cond-mat/ 0506462.

²C. J. Umrigar and X. Gonze, Phys. Rev. A **50**, 3827 (1994).

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