Developing an empirical Laplacian-based model for the exchange-correlation energy.

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We report recent work in developing a GGA-quality 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 atom[1]. A comparison of our data to a more popular candidate for building DFT's, the kinetic energy density, reveals that while the KE density is a reasonable candidate for fitting the data, it is not as good as the Laplacian, failing primarily in the covalent bond. Preliminary tests of the Laplacian 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. An all-electron generalization of the model is constructed by consideration of the cusp in the electron density at the nucleus. The use of $\nabla^2 n$ trivially avoids the singularity in the Kohn-Sham potential that gradient-based models suffer at the nucleus due to this cusp but tends to generate large oscillations elsewhere.

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