Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Beyond the LDA in density functional theory: empirical Laplacian-based models for the exchange-correlation energy[1] ANTONIO C. CANCIO, CHRISTOPHER E. WAGNER, Ball State University — We report recent work in developing a GGA-level density functional theory using primarily the Laplacian of the density $\nabla^2 n$ as an input beyond the LDA. Our starting point and motivation is a model fit to the exchange-correlation energy density of the valence shell of the Si crystal and other systems, as calculated by quantum Monte Carlo simulations, which show a strong, roughly linear dependence of this quantity on the Laplacian. The model respects the Lieb-Oxford bound for large positive Laplacian but suffers from a pole at negative values. A better treatment of $\nabla^2 n$ in this limit can be used to construct an all-electron extension of our model, and as an added benefit, avoid 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 fit exchange energy densities in the cusp region accurately; obtaining reasonable potentials is a harder task but made easier by keeping the gradient of the density.

[1]Work support by National Science Foundation grant DMR-0812195.

Antonio C. Cancio
Ball State University

Date submitted: 27 Nov 2010 Electronic form version 1.4