Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Laplacian-based generalized gradient approximations for the exchange energy[1] A.C. CANCIO, Ball State University, CHRIS E. WAGNER, University of Florida — It is well known that in the gradient expansion approximation to density functional theory (DFT) the gradient and Laplacian of the density make interchangeable contributions to the exchange-correlation (XC) energy. This is an arbitrary "gauge freedom" for building DFT models, normally used to eliminate the Laplacian from the generalized gradient approximation (GGA) level of DFT development. We explore the implications of keeping the Laplacian at this level of DFT, in order to develop a model that fits the known behavior of the XC hole, which can only be described as a system average in a conventional GGA. We generate a family of exchange models that obey the same constraints as conventional GGA's, but which in addition have a finite-valued potential at the atomic nucleus unlike GGA's. These are tested against exact densities and exchange potentials for small atoms and finite jellium drops, and for constraints chosen to reproduce the PBEsol and the APBE variants of the GGA. We find that exchange energies of atoms can be reliably reproduced, by breaking the local (but not global) Lieb-Oxford bound.

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

Antonio C. Cancio
Ball State University

Date submitted: 12 Dec 2012 Electronic form version 1.4