Abstract Submitted
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Exploring the Dependence of the Exchange-Correlation Energy on the Laplacian of the Electron Density SETH ROSS, A.C. CANCIO, Ball State University — It has been observed that the deviation of exchange-correlation (XC) energy from the local density approximation (LDA) model in quantum Monte Carlo simulations of several systems correlates to the local Laplacian of the density [1] in a roughly linear fashion. We examine the effects on the prediction of typical material properties of the linear dependence of the XC energy density on the Laplacian of the density. To do this we focus on slowly varying systems within LDA and generalized gradient approximation models and compare these models using the Laplacian. We use the pseudopotential code Abinit to examine selected systems such as the AE6 test set and some typical solids such as Si, Cu, Na and NaCl. We then observe the differences between predictions of properties, particularly atomization energies and bond lengths of molecules and cohesive energies and lattice constants of solids, between standard DFT models and models using the Laplacian.

[1] A. C. Cancio and M. Y. Chou, Phys. Rev. B. 74, 081202 (2006)

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