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Revisiting the GGA in density functional theory: Laplacian-based models for the exchange-correlation energy[1] ANTONIO C. CANCIO, CHRISTOPHER E. WAGNER[2], 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, such as exist near an atomic nucleus. 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. We develop and test out an optimization method to minimize unwanted oscillations in the potential that can be a hazard with DFT's that use the Laplacian.

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[2]currently at University of Florida

Antonio C. Cancio
Ball State University

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