ABSTRACT

THESIS: Visualization of orbital free models of kinetic energy density in solids

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The metaGGA class of functionals for describing the exchange-correlation (XC) energy in density functional theory (DFT) is conventionally constructed as a functional dependent on the density, density gradient, and kinetic energy density (KED). The addition of the KED makes metaGGAs more accurate functionals than ones that use the density and its gradient alone but also more computationally expensive for some applications such as ab initio molecular dynamics simulations. The calculation of the XC energy in metaGGAs can be made less expensive by replacing the explicit orbital dependence in the KED with expressions involving only the particle density and its gradient and Laplacian. We test the validity of recent deorbitalization strategies in the literature by visualizing their predictions for the KED and related quantities, and comparing these to exact calculations. For an effective test, we perform these calculations on semiconductor solids with varying ionicity and atomic number. We explore how well the KED can be represented by a single metaGGA model in terms of the scaled gradient, Laplacian of the density, and scaled density. The results show a near-universal linear correlation with Laplacian and gradient for regions outside of the atomic bond, which can be fit to a straight line when viewed at the optimal rotation. The calculations of exact KED and electron density are done with the ABINIT DFT plane-wave pseudopotential code.