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Visualizing the Kohn-Sham kinetic energy density in molecules[1]

ANTONIO C. CANCIO, AERYK KUNA, Ball State University — In recent years, driven by applications at high temperature and large system size, interest has turned to the construction of orbital-free density functionals, modeling the kinetic energy solely as a functional of the electron density and its derivatives. We visualize the Kohn-Sham kinetic energy density (KED) for the AE6 test set of molecules commonly used to test density functional performance for atomization energies. Calculations are performed using the ABINIT plane-wave code with over-converged cutoffs and simulation cell sizes to produce as accurate results as possible within a pseudopotential approximation. The orbital-dependent KED is compared to simple orbital-free models such as the Thomas-Fermi and von-Weiszacker KED's and to a sophisticated metaGGA-level functional proposed by Perdew and Constantin (PC). All models fail to reproduce the Kohn-Sham KED reasonably in high density regions – covalent and polar bonds and valence lone-pairs. In particular, the PC model actually disimproves on the simpler gradient expansion model in these regions. A simple fix is proposed for the PC functional, substantially modifying its behavior for regions of high values of the Laplacian of the density and low density gradient.

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