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Modeling the kinetic energy density of molecules – towards an orbital-free meta-GGA ANTONIO CANCIO, DANE STEWART, JEREMY REDD, Ball State University — Driven by applications at high temperature and large system size, interest has recently turned to the construction of orbital-free density functionals, modeling the Kohn-Sham kinetic energy solely as a functional of the electron density and its derivatives. We report work on a metaGGA level orbital-free kinetic energy functional parametrized in terms of the local Laplacian and gradient of the density, and based on insights gained in the visualization of the kinetic energy density (KED) for atoms and the AE6 test set of molecules. Visualization of the KED, particularly in the region of localized electron pairs, such as atomic lone pairs and covalent bonds, pointed out significant flaws in an earlier metaGGA proposed by Perdew and Constantin. We find that these can be substantially fixed by revising an implicit constraint built into the prior model in the limit of strong electron localization – when the Kohn-Sham KED approaches the bosonic limit. A first attempt at an improved model dramatically improves atomization energies for the AE6 test set, but remains an order of magnitude worse than a conventional Kohn-Sham GGA. We are currently working to fix a notable overcorrection of the PC meta-GGA for the electron localization limit that may lead to further improvement.

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