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Fitting of Molecular Densities by Compact, Atom-Centered Expansion[1] V.V. KARASIEV, S.B. TRICKEY, FRANK E. HARRIS[2], Quantum Theory Project and Dept. of Physics, U. of Florida — Use of an orbital-free (OF) version of DFT requires both a suitable approximate Kohn-Sham kinetic energy functional and a systematic but simple model of the system density. We report useful approximations to the KS density via a very compact expansion in atom-centered functions. Spherically averaged, isolated-atom densities are used as basis functions to expand spherically symmetric atom-centered contributions. A simplified expansion in real spherical harmonics is then added to the spherically symmetric contributions. Although drastically simplified, such representations of the density nevertheless result in impressively small mean square deviations relative to the target KS density. The fitted density can then be combined with an approximate OF-KE functional we have developed [3] to generate energy surfaces. These energy surfaces have shapes similar to those arising from true KS densities, and are therefore suitable for calculation of forces to drive molecular dynamics simulations.

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[3]V.V. Karasiev, S.B. Trickey, and F.E. Harris, J. Comp. Aided Mat. Des. (2005) (accepted).

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