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Orbital-free density functional theory with atom-centered density matrices

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Orbital-free density functional theory (OFDFT) is one of the most computationally efficient methods for performing electronic structure calculations. It employs an explicit density functional $T_s[n]$ to approximate the kinetic energy of non-interacting electrons, bypassing any requirement for single particle orbitals. The lack of wave-function manipulations allows OFDFT calculations to scale quasi-linearly with system size, with a small prefactor.

Conventional OFDFT utilizes the electron density as the sole working variable. This poster will explore a modification to the usual approach that introduces on-site density matrices. The local density matrices are defined only in spheres immediately surrounding nuclei, and the remainder of the system is described by the electron density alone. This hybrid description affords possible improvements in both accuracy and computational efficiency.