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Nonlocal Kinetic Energy Functional Enables Reliable Large-scale Electronic Structure Simulations WENHUI MI, MICHELE PAVANELLO, Department of physics chemistry, Rutgers University, Newark, NJ07012 — Orbital-Free DFT (OF-DFT) and subsystem DFT (sDFT) are two promising approaches for large-scale electronic structure simulations, owing to their computational cost is linear scaling with system size. The common central ingredient of these two approaches is the kinetic energy functional (KEDF) which determines the accuracy of the performance. Unfortunately, with the available KEDFs, systems having highly inhomogeneous electron densities still fall outside OF-DFT's range of applicability. In sDFT, Currently employed KEDFs are at most semi-local, and simulations only included systems composed of weakly interacting subsystems. Recently, we made considerable progress in addressing this problem by proposing a new generation of nonlocal KEDFs that features correct asymptotic and ability to handle highly inhomogeneous electron densities. With these KEDFs, OF-DFT achieves close to chemical accuracy for the electronic energy for quantum dots and metal clusters. Benchmarks for the various bonded systems show that the new nonlocal sDFT considerably improves the computed interaction energies and electron densities compared to commonly employed (semi) local sDFT. Our work shows that the new generation of nonlocal KEDF enables both OF-DFT and sDFT for reliable large-scale simulations.

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