A Generalized Gradient Approximation for the Non-interacting Kinetic Energy Density Functional Adapted to Pseudo-densities

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Reliable and accurate approximation of the non-interacting kinetic energy density functional (KEDF) remains a challenge for extensive usage of orbital-free density functional theory (OF-DFT). A major potential OF-DFT application is inexpensive calculation of the electronic forces in {\it ab initio} molecular dynamics (AIMD). We propose a novel generalized gradient approximation (GGA) non-interacting KEDF for use in the context of ab initio molecular dynamics (AIMD). In AIMD, pseudo-potentials are used ubiquitously and the associated pseudo-densities by construction have properties distinct from physical densities. The sole parameter in the new functional is determined by imposition of the rigorous Pauli potential positivity constraint for pseudo-atoms at postscf level. In static lattice tests on simple solids the new functional outperforms the previous best constraint-based single-point functional, VT84F (Phys. Rev. B \textbf{88}, 161108(R) (2013)). VT84F satisfies the positivity constraint for Kato densities but not pseudo-densities. The new functional also does quite well in comparison with parametrized two-point functionals.

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