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Orbital-free Kinetic Energy Density Functionals of GGA Type with Positive-definite, Finite Pauli Potentials[1] S.B. TRICKEY, QTP, Univ. Florida, V.V. KARASIEV, Instituto Venezolano de Investigaciones Cientificas, R.S. JONES, Physics, Loyola College of Maryland, FRANK HARRIS, Physics, Univ. Utah — A reliable, orbital-free expression for the Kohn-Sham kinetic energy functional T_s would provide Born-Oppenheimer forces for first-principles molecular dynamics with a computational cost scaling as the relevant system volume rather than some power of the electron count N_e. In previous work (J. Computer-Aided Mat. Des. **13**, 111 (2006)) we obtained improved (compared to published) generalized gradient approximate KE functionals by requiring positive-definiteness of the Pauli potential, $v_\theta = \delta T_\theta / \delta n$, with $T_s = T_w + T_\theta$ and T_w the von Weizsäcker KE functional. However, such modified conjoint functionals still generate unphysical singularities at the nuclei. Here we discuss a systematic use of gradient expansion truncations to generate constrained enhancement factors for GGA functionals that are guaranteed to yield v_θ that is both everywhere positive definite and finite at the nuclei. Illustrative results will be reported.

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