# Constraint-based Parmeterization of Reduced Derivative Approximation Kinetic Energy Functionals

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Use of orbital-free DFT dramatically accelerates evaluation of forces in ab-initio MD at any temperature [1]. Recently we have achieved a fully non-empirical constraint-based generalized gradient (GGA) [2] functional for the non-interacting kinetic energy which gives both reasonable ground-state binding and reasonable pressure errors over a large range of temperatures. A limitation of the GGA form, the inescapable presence of nuclear site singularities in the KE potential, motivates a further step. Inclusion of higher-order spatial derivatives of the density in the form of reduced density derivatives (RDDs) [3] adds flexibility to the functional form for meeting constraints but requires new design criteria. Specifically, the reduced derivative approximation (RDA) functionals, which use RDD variables, provide a positive-definite Pauli potential which is non-singular near nuclei. Here we focus on such higher-order derivative combinations to design a non-empirical, constraint-based RDA [3-5] functional and report our progress on that agenda.

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