

A PW91-like exchange with a simple analytical form

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A pair of families of generalized gradient approximation (GGA) exchange functionals is presented. The aim is to simplify the PW91 enhancement function considerably, yet retain its shape, not affect its performance and, perhaps, even improve on it. The functionals are constructed non-empirically taking as kernels the PBE and RPBE analytic forms and adding a Gaussian tail to incorporate satisfaction of the asymptotic reduced-gradient constraint from non-uniform scaling. The standard heats of formation are considerably improved by the functionals proposed in this Letter compared to PBE or even PBE-LS (our best previous functional). Barrier heights are marginally improved and there are no significant quality losses. Globally, the new functionals exhibit much better balance in predicting thermodynamic and kinetic properties than any competing GGA. This work belongs to our ongoing research of exploring the role of constraints in exchange-correlation functional design.¹⁻⁶

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