Meta-generalized gradient approximation: Third rung on the ladder of density functional approximations

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On the Jacob’s Ladder of density functional approximations to the exchange-correlation energy, each higher rung adds another local ingredient which can be used to satisfy further exact constraints. The first rung is the local density approximation. The second rung or generalized gradient approximation (GGA) adds the gradient of the density. The third rung or meta-GGA further adds the Kohn-Sham orbital kinetic energy density. I will review the nonempirical construction of a recent meta-GGA [1] and its mostly-successful numerical tests for molecules [2,3] and solids [4].


