Meta-generalized gradient approximations in density functional theory

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One of the challenges in density functional theory (DFT) is to improve the accuracy of its exchange-correlation functional, the only part to be approximated, while maintaining computational efficiency. On the Jacob's ladder categorizing the approximations based on their inputs to the exchange-correlation energy density, higher rungs are usually built on and thus improve accuracy over lower ones. However, climbing from the lowest three semilocal rungs [local spin density approximation (LSDA), generalized gradient approximation (GGA), and meta-GGA (MGGA)] to the higher fully-nonlocal rungs usually increases the computational cost dramatically. MGGA is the highest and potentially most accurate semilocal rung of the Jacob's ladder, which includes as an input the kinetic energy density in addition to the electron density and its gradient used in GGAs. I will show that the inclusion of the kinetic energy density enables MGGA to recognize different chemical bonds (covalent, metallic, and even weak ones) and assign different GGA descriptions for different bonds. I further show that better nonlocal functionals can be constructed based on a better semilocal one (e.g., global hybrid MGGA vs. global hybrid GGA). I will also discuss a bound on the exchange energy that can be built into MGGAs but is incompatible with GGAs.