Effect of the orbital-overlap dependence on Meta Generalized Gradient Approximation

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The dimensionless inhomogeneity parameter, $\alpha$, characterizing the extent of orbital overlap, is disentangled for the first time, by the means of separability assumption, from the other dimensionless inhomogeneity parameter, $s$, the reduced density gradient, in terms of constructing a meta generalized gradient approximation (MGGA) for the exchange functional. We show that the formation of the intershell region in an atom is associated with increase of $\alpha$. This observation leads to a simple nonempirical MGGA exchange functional, which interpolates between the single-orbital regime for confinement systems, where $\alpha = 0$, and the slowly varying density regime, where $\alpha \approx 1$, and then extrapolates to $\alpha \to \infty$. The simple MGGA exchange functional penalizes the formation of the intershell region by having monotonically increasing $s$-dependence and monotonically decreasing $\alpha$-dependence. When it is combined with the variant of the Perdew-Burke-Erzerhof (PBE) GGA correlation as used in the revised Tao-Perdew-Staroverov-Scuseria (revTPSS) MGGA, the resulted MGGA performs equally well for atoms, molecules, surfaces, and solids, with an implication of a tight Lieb-Oxford bound.