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Effect of the orbital-overlap dependence on Meta Generalized Gradient Approximation JIANWEI SUN, JOHN PERDEW, BING XIAO, ADRIENN RUZSINSZKY, Department of Physics and Engineering Physics, Tulane University — The dimensionless inhomogeneity parameter, α, characterizing the extent of orbital overlap, is disentangled 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 inside an atom is associated with increase ofα, which suggests MGGA should expect a monotonically decreasing α dependence for a wide range of density. This leads to a simple nonempirical MGGA exchange functional, which interpolates between the sigle-orbital regime for confinement systems, where α=0, and the slowly varying density regime, where $\alpha \approx 1$, and then extrapolates to $\alpha \to \infty$. The new MGGA exchange functional, combined with the variant of the Perdew-Burke-Erzerhof (PBE) GGA correlation as used in the revised Tao-Perdew-Staroverov-Scuseria (revTPSS) MGGA [1], performs equally well for atoms, molecules, surfaces, and solids, with an implication of a tight Lieb-Oxford bound.

[1] J.P. Perdew, A. Ruzsinszky, G.I. Csonka, L.A. Constantin, and J. Sun, Phys. Rev. Lett. 103, 026403 (2009).

Jianwei Sun
Department of Physics and Engineering Physics, Tulane University

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