

MAR10-2009-003803

Abstract for an Invited Paper  
for the MAR10 Meeting of  
the American Physical Society

**Meta-generalized gradient approximations: What they can and cannot do for you<sup>1</sup>**

JOHN P. PERDEW, Department of Physics, Tulane University, New Orleans, LA 70118

In the meta-GGA, as first proposed by Becke, the exchange-correlation energy is expressed as a single integral over position space of a function of the electron density, its gradient, and the orbital kinetic energy density of Kohn-Sham density functional theory. Meta-GGA is the highest level of semilocal (hence computationally efficient) approximation. Like the simpler GGA, it can be constructed nonempirically [1,2] by constraint satisfaction. But, unlike the GGA, it is capable of high simultaneous accuracy for atoms and molecules on the one hand and solids on the other, because it provides different GGA descriptions in regions where one orbital shape dominates and where all orbitals overlap strongly. A good meta-GGA may work in all situations where the exact exchange-correlation hole is well-localized around its electron (atoms, slowly-varying densities, many molecules and solids near equilibrium). But it will necessarily fail to the extent that the exact exchange-correlation hole is delocalized, as in many stretched-bond situations or where long-range van der Waals effects are important. While full nonlocality is needed to describe the latter situations, the meta-GGA appears to be otherwise a good compromise between accuracy and efficiency. Further improvements to the meta-GGA may still be possible. Selfconsistent meta-GGA's are increasingly available in standard codes for atoms, molecules, and solids. [1] J. Tao, J.P. Perdew, V.N. Staroverov, and G.E. Scuseria, Phys. Rev. Lett. 91, 146401 (2003). [2] J.P. Perdew, A. Ruzsinszky, G.I. Csonka, L.A. Constantin, and J.Sun, Phys. Rev. Lett. 103, 026403 (2009).

<sup>1</sup>Supported by NSF.