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Toward Improved Semilocal and Nonlocal Density Functionals for Atoms, Molecules, and Solids[1]

JOHN P. PERDEW, Tulane University

Semilocal density functionals construct the exchange-correlation energy density at a point from the electron density and orbitals in the neighborhood of that point. They can be constructed nonempirically, and work best for sp-bonded systems near equilibrium. They increase in sophistication from the local spin density approximation to the generalized gradient approximation to the meta-GGA. For a molecule like CO on a transition metal surface, it appears that only a meta-GGA can give a good simultaneous description of the lattice constant and surface energy of the metal, on the one hand, and the adsorption energy of the molecule on the other [1]. I will discuss two remaining deficiencies of the revised TPSS meta-GGA [2]: its artificial order-of-limits problem, and its need for more information about non-bonded interaction. When electrons are shared over stretched bonds, full nonlocality is needed, and typically empirical parameters are also needed. This suggests that we don't yet know enough about the full nonlocality of the density functional for the exchange-correlation energy.

[1] J. Sun, M. Marsman, A. Ruzsinszky, G. Kresse, and J.P. Perdew, Phys. Rev. B 83, 121410 (2011).
[2] J.P. Perdew, A. Ruzsinszky, G.I. Csonka, L.A. Constantin, and J. Sun, Phys. Rev. Lett. 103, 026403 (2009).

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