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Restoring the Density-Gradient Expansion for Exchange in a GGA for Solid and Surfaces[1]

JOHN P. PERDEW, Department. of Physics and Quantum Theory Group, Tulane University, New Orleans, LA 70118

Density functionals for the exchange-correlation energy of a many-electron system are widely used in condensed-matter physics. Successful modern generalized gradient approximations (GGA's), developed largely for quantum chemistry, are biased toward free-atom energies. Recent "GGA's for solids" include PBEsol [1], a revised Perdew-Burke-Ernzerhof (PBE) GGA that improves equilibrium properties of densely-packed solids and their surfaces by recovering the first-principles density-gradient expansion for the exchange energy [2]. Results will be reported for the lattice constants of 20 solids and for the surface energy of jellium in the local spin density approximation and in the PBE and PBEsol GGA's. Other possible applications of PBEsol will be discussed. It will be argued (as in Ref. [3]) that the second-order gradient expansion is nearly converged for exchange, but not for correlation, in valence regions of typical solids (while atoms require a larger gradient coefficient for exchange).

[1] J.P. Perdew, A. Ruzsinszky, G.I. Csonka, O.A. Vydrov, G.E. Scuseria, L.A. Constantin, X. Zhou, K. Burke, http://arxiv.org/abs/0711.0156

[2] P.R. Antoniewicz and L. Kleinman, Phys. Rev. B **31**, 6779 (1985).

[3] J.P. Perdew, L.A. Constantin, E. Sagvolden, and K. Burke, Phys. Rev. Lett. **97**, 223002 (2006).

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