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Strongly Constrained and Appropriately Normed (SCAN) Meta-Generalized Gradient Approximation for Exchange and Correlation[1]

JIANWEI SUN, ADRIENN RUZSINSZKY, JOHN PERDEW, Department of Physics, Temple University — Meta-generalized gradient approximations (meta-GGAs) construct the exchange-correlation (xc) energy density from the local electron density, its gradient, and the orbital kinetic energy density. They are the most accurate of the computationally-efficient semilocal density functionals. We construct a SCAN meta-GGA which satisfies all the known exact constraints that a meta-GGA can, including a new tight lower bound on the exchange energy [1]. SCAN is constructed as an interpolation/extrapolation on α, the dimensionless variable that can recognize covalent single ($\alpha \approx 0$), metallic ($\alpha \approx 1$), and weak ($\alpha >> 1$) bonds [2]. A few parameters are included for appropriate norming on systems where a meta-GGA should be especially accurate due to xc hole localization.

[1] J.P. Perdew, A. Ruzsinszky, J. Sun. and K. Burke, J. Chem. Phys. 140, 18A533 (2014).
[2] J. Sun et al., Phys. Rev. Lett. 111, 106401 (2013).

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