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Quenched Lieb-Oxford Satisfaction and Improved Performance for PBE-type Functionals[1] S.B. TRICKEY, QTP, Univ. Florida, V. MEDEL, A. VELA, Cinvestav, Mexico City — Success for the orbital-free DFT approach to Born-Oppenheimer forces for first-principles molecular dynamics requires progress on orbital-free exchange-correlation (XC) functionals to go along with newly developed orbital-free kinetic energy functionals [V.V. Karasiev *et al.* arXiv 0809.4798, J. Comput.-Aided Mat.Des. **13**, 111 (2006)]. We report on development and testing of a non-empirical X functional which generalizes PBE X. It satisfies a reduced Lieb-Oxford bound by quenching to homogeneous electron gas behavior for large values of the inhomogeneity $s \propto |\nabla n|/n^{4/3}$ on the grounds that large s often corresponds (counter-intuitively) to small, smooth density. Used with the PBE C functional, our X functional reduces mean absolute errors for small molecules by 20% or more with respect to conventional PBE XC. Used with LYP C (a semi-empirical combination), the performance also is improved relative to PBE-LYP.

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Sam Trickey
Univ. of Florida

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