Advances in Local Hybrid Functionals

ALEXEY ARBUZNIKOV, MARTIN KAUPP, HILKE BAHMANN, University of Wuerzburg — Local hybrids\(^1\) provide a promising new generation of exchange-correlation functionals for the simultaneous accurate description of various properties (atomization energies, reaction barrier heights,\(^2\) NMR chemical shifts,\(^3\) energetics of transition-metal systems, etc.) Compared to traditional (global) hybrids (e.g., B3LYP), instead of a constant exact-exchange admixture, local hybrids employ a position-dependent one. The latter is governed by a so-called *local mixing function* (LMF), and this is the crucial quantity controlling the performance of local hybrids. Here we present and compare new results obtained with LMFs derived both in a semiempirical way and using *ab initio* considerations, e.g., the adiabatic connection formalism.\(^4\) The former approach yields better results, while the latter brings valuable insights into the performance and limits of local hybrids.

\(^1\)Jaramillo, J; Scuseria, G. E.; Ernzerhof, M. *J. Chem. Phys.* 2003, 118, 1068
\(^3\)Arbuznikov, A. V.; Kaupp, M. *Chem. Phys. Lett.* 2007, 442, 496