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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
[2]Kaupp, M.; Bahmann, H.; Arbuznikov, A. V. *J. Chem. Phys.*, **2007**, 127, 194102
[3]Arbuznikov, A. V.; Kaupp, M. *Chem. Phys. Lett.* **2007**, 442, 496
[4]Arbuznikov, A. V.; Kaupp, M. *J. Chem. Phys.* **2008**, 128, 214107

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