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NSF research by Yan Zhao and Don Truhlar

Density functional theory is widely used in the computational chemistry community, but the most popular density functional, B3LYP, has some serious shortcomings: (i) it is better for main-group chemistry than for transition metals; (ii) it systematically underestimates reaction barriers; (iii) it is inaccurate for interactions dominated by medium-range correlation energy, such as van der Waals attraction, aromatic–aromatic stacking, and alkane isomerization energies. We developed new functionals that overcome these difficulties: (a) M06, a hybrid meta_GGA functional, is a functional with good accuracy "across-the-board" for transition metals, main group thermochemistry, medium-range correlation energy, and barrier heights. (b) M06–2X, M08-HX, and M08-SO. which are also hybrid meta-GGAs, have excellent performance for main group chemistry, predicts accurate valence and Rydberg electronic excitation energies, and are excellent functional for aromatic–aromatic stacking interactions. (c) M06–L is not as accurate as M06 for barrier heights but is the most accurate functional for transition metals and is the only local functional (no Hartree-Fock exchange) with better across-the-board average performance than B3LYP; this is very important because only local functionals are affordable for many demanding applications on very large systems.

"Density Functionals with Broad Applicability in Chemistry," Y. Zhao and D. G. Truhlar, Accounts of Chemical Research **41**, 157-167 (2008).

"Applications and Validations of the Minnesota Density Functionals," Y. Zhao and D. G. Truhlar, Chemical Physics Letters **502**, 1-13 (2010). (Frontiers Article)

Application areas of the Minnesota density functionals