

What's New in Q-Chem

Feature 14

Double-Hybrid Density Functional Theory

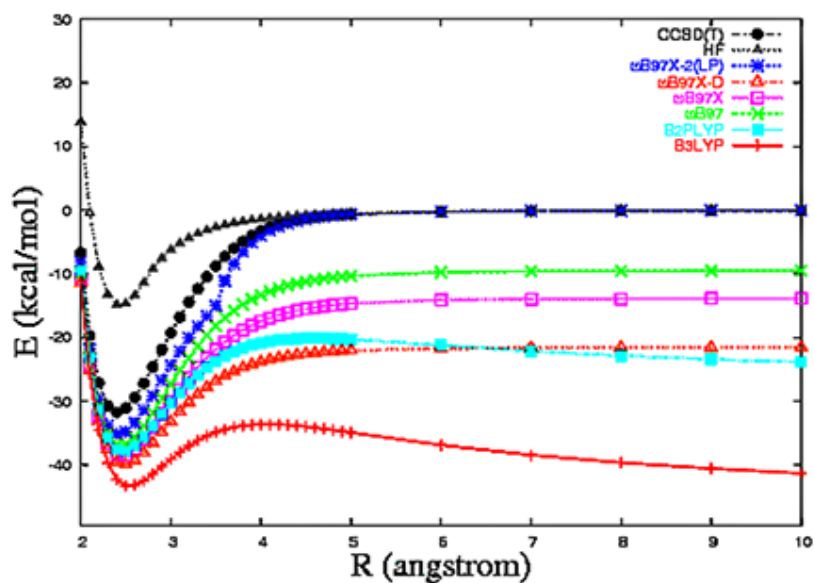
Developers: Jeng-Da Chai

Double-hybrid density functional theory has shown a great promise in approaching the chemical accuracy with a computational cost similar to MP2. Unlike traditional KS-DFT approaches, double-hybrid DFT can perform well in both noncovalent and covalent systems.

Figure to the right: Dissociation curve of Ar_2^+ . Zero level is set to $E(\text{Ar}) + E(\text{Ar}^+)$ for each method.

As shown, self-interaction errors are greatly reduced by $\omega\text{B97X-2}$, when compared with several hybrid (and double-hybrid) density functionals.

(figure taken from J.-D. Chai and M. Head-Gordon, *J. Chem. Phys.* 131, 174105 (2009))



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www.q-chem.com/whatsNew4.html

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Double-Hybrid Density Functional Theory (continued)



Publications:

[S. Grimme, "Semiempirical hybrid density functional with perturbative second-order correlation," J. Chem. Phys. 124, 034108 \(2006\)](#)

[T. Schwabe and S. Grimme, "Double-hybrid density functionals with long-range dispersion corrections: higher accuracy and extended applicability," Phys. Chem. Chem. Phys. 9, 3397 \(2007\)](#)

[Y. Zhang, X. Xu, W. A. Goddard III, " Doubly hybrid density functional for accurate descriptions of nonbond interactions, thermochemistry, and thermochemical kinetics ", PNAS 106, 4963 \(2009\)](#)

[J.-D. Chai and M. Head-Gordon, " Long-Range Corrected Double-Hybrid Density Functionals ", Phys. 131, 174105 \(2009\)](#)

For more information on how to use this feature, refer to the [Q-Chem Manual, Section 4.3.8](#)

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