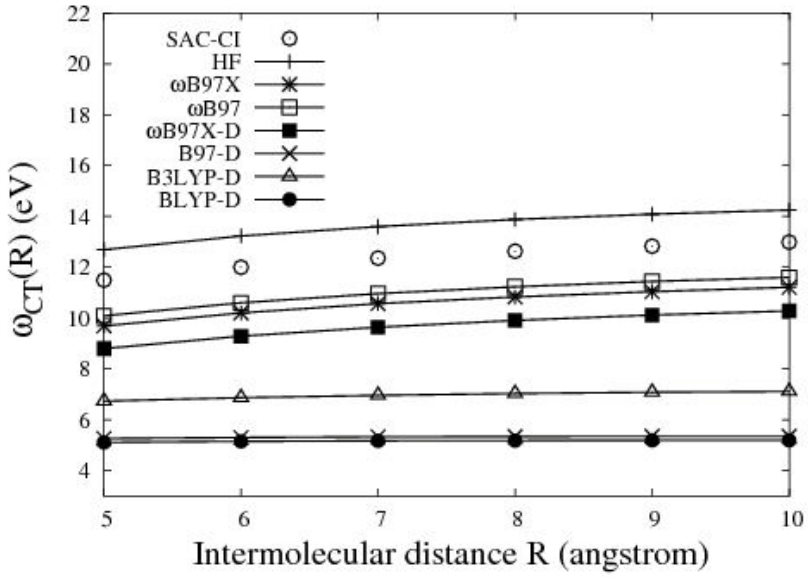
What's New in Q-Chem

Feature 13

A Family of Long-Range Corrected Hybrid Functionals: wB97, wB97X, wB97X-D, wB97X-2

Developers: Jeng-Da Chai, Yihan Shao (for analytical Hessians)

It has been demonstrated that self-interaction errors (SIE) can be greatly reduced by long-ranged corrected (LRC) hybrid density functional theory, which includes a full Hartree-Fock exchange at long-range interelectron distance. Chai and Head-Gordon developed a family of wB97 series for general applications: systems with serious SIE issues, thermochemistry, thermal kinetics, noncovalent systems, and time-dependent DFT. Unlike KS-GGAs or global hybrid functionals, this wB97 series, optimized with a systematic procedure, has shown a great promise for general applications.



The graph to the left (taken from Ref. 2) shows an overall excellent performance of wB97 series in predicting long-range charge-transfer excitations of two well-separated molecules (C_2H_4 and C_2F_4).

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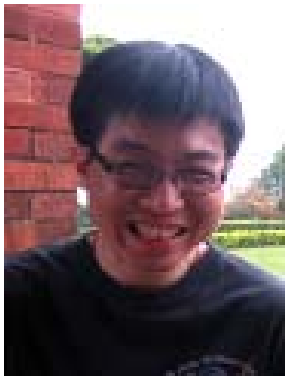
What's New in Q-Chem

A Family of Long-Range Corrected Hybrid Functionals: wB97, wB97X, wB97X-D, wB97X-2 (continued)



Jeng-Da Chai

Publications:

J.-D. Chai and M. Head-Gordon, "Systematic Optimization of Long-Range Corrected Hybrid Density Functionals"
J. Chem. Phys. 128, 084106 (2008)

J.-D. Chai and M. Head-Gordon, "Long range corrected hybrid density functional with damped atom-atom dispersion corrections." Phys. Chem. Chem. Phys. 10, 6615 (2008)

J.-D. Chai and M. Head-Gordon, "Optimal Operators for Hartree-Fock Exchange from Long-Range Corrected Hybrid Density Functionals."
Chem. Phys. Lett. 467, 176 (2008)

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

For more information on how to use this feature, refer to the Q-Chem Manual, Section 4.3.4.3.

For more new features, visit:
www.q-chem.com/whatsNew4.html

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