Chemistry Central Journal

Poster presentation

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Latest developments and applications of double-hybrid density functionals

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from 3rd German Conference on Chemoinformatics
Goslar, Germany. 11-13 November 2007

Published: 26 March 2008

Chemistry Central Journal 2008, **2**(Suppl 1):P47 doi:10.1186/1752-153X-2-S1-P47

This abstract is available from: http://www.journal.chemistrycentral.com/content/2/S1/P47

The neglect of non-local electron correlation effects is a serious drawback of common DFT methods. To remedy this, we have recently developed double-hybrid density functionals (X2PLYP family) [1,2], which add a second order perturbation correction for correlation to a standard hybrid functional in an empirical way.

Here we give an overview of the extensions of our previous work. We discuss the analytical gradient for structure optimisations [3], the combination with an empirical dispersion correction (DFT-D) [4], and the computation of excitation energies in a time-dependent framework [5]. We present results for several benchmark sets and for some challenging applications. In all cases very accurate results are obtained at a reasonable computational expense. These show, that our method outperforms common (TD)DFT approaches and is even competitive to more sophisticated approaches like CCSD(T).

References

1. Grimme S: *J Chem Phys* 2006, **124:**34108.
2. Schwabe T, Grimme S: *Phys Chem Chem Phys* 2006, **8:**4398.
3. Neese F, Schwabe T, Grimme S: *J Chem Phys* 2007, **126:**124115.
4. Schwabe T, Grimme S: *Phys Chem Chem Phys* 2007, **9:**3397.
5. Grimme S, Neese F: *J Chem Phys* 2007, **127:**154116.