Explicitly Correlated Multireference Electronic Structure Methods

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Recent developments of multireference electron correlation methods in our group are reviewed. In particular, we will focus on new explicitly correlated multireference perturbation theory and multireference configuration interaction methods [1,2]. The explicitly correlated (F12) terms very much reduce the basis set incompleteness errors, and typically at least quintuple-zeta quality is achieved already with triple-zeta basis sets. The additional cost is negligible. Benchmarks are presented for ground and excited states and various properties of molecules and elementary reactions. Furthermore, new implementations of analytic energy gradients for state-averaged CASSCF and CASPT2 wave functions [3] that employ density fitting techniques to speed-up the evaluation of the two-electron integrals are presented. Finally, some applications to open-shell transition metal complexes with complicated electronic structure are discussed.

[1] K. R. Shamasundar, G. Knizia, and H.-J. Werner, J. Chem. Phys. **135**, 054101 (2011).
[2] For a review and further references see: T. Shiozaki and H.-J. Werner, Mol. Phys. **111**, 607 (2013).
[3] W. Györffy, T. Shiozaki, G. Knizia, and H.-J. Werner, J. Chem. Phys. **138**, 104104 (2013).