

## Publikationsliste Helmich-Paris, Stand: 29.04.2021

1. B. Helmich-Paris; A trust-region augmented Hessian implementation for restricted and unrestricted Hartree-Fock and Kohn-Sham methods. *J. Chem. Phys.*, 154 (16), 164104 (2021)
2. B. Helmich-Paris; Simulating X-ray absorption spectra with CASSCF linear response methods *Int. J. Quantum Chem.*, e26559 (2020).
3. T. Saue et al.; The DIRAC code for relativistic molecular calculations. *J. Chem. Phys.* 152 (20), 204104 (2020).
4. S. G. Balasubramani et al.; TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations *J. Chem. Phys.* 152 (18), 184107 (2020).
5. B. Helmich-Paris; Benchmarks for Electronically Excited States with CASSCF Methods. *J. Chem. Theory Comput.*, 15, 4170-4179 (2019).
6. B. Helmich-Paris; CASSCF linear response calculations for large open-shell molecules. *J. Chem. Phys.* 150 (17), 174121 (2019).
7. C. Kollmar; K. Sivalingam; B. Helmich-Paris; C. Angeli; F. Neese. A perturbation-based Super-CI approach for the orbital optimization of a CASSCF wave function. *J. Comput. Chem.* 40 (14), 1463-1470 (2018).
8. B. Helmich-Paris; M. Repisky; L. Visscher. Relativistic Cholesky-decomposed density matrix MP2 for large molecules. *Chem. Phys.* 518, 38-46 (2019).
9. C. Badala Viswanatha; B. Helmich-Paris; C. Hättig. Circularly polarized fluorescence and phosphorescence calculations on organic molecules using the approximate coupled-cluster model CC2, *Phys. Chem. Chem. Phys.* 20; 21051–21061 (2018).
10. B. Helmich-Paris; C. Hättig; C. van Wüllen. Correction to Spin-Free CC2 Implementation of Induced Transitions between Singlet Ground and Triplet Excited States. *J. Chem. Theory Comput.* 13, 3426-3426 (2017).
11. B. Helmich-Paris; S. Knecht. Laplace-transformed multi-reference second-order perturbation theories in the atomic and active molecular orbital basis *J. Chem. Phys.* 146, 224101 (2017).
12. B. Helmich-Paris; M. Repisky; L. Visscher. Laplace-transformed atomic orbital-based Møller–Plesset perturbation theory for relativistic two-component Hamiltonians. *J. Chem. Phys.* 145, 014107 (2016).
13. B. Helmich-Paris; L. Visscher. Improvements on the minimax algorithm for the Laplace transformation of orbital energy denominators *J. Comput. Phys.* 321, 927–931 (2016).
14. B. Helmich-Paris; C. Hättig; C. van Wüllen. Spin-Free CC2 Implementation of Induced Transitions between Singlet Ground and Triplet Excited States. *J. Chem. Theory Comput.* 12, 1892–1904 (2016).
15. B. Helmich. Paarspezifische natürliche Orbitale zur effizienten Berechnung von Coupled-Cluster-Anregungsenergien. Ph.D. thesis, Ruhr-Universität Bochum, (2014).
16. B. Helmich; C. Hättig. A pair natural orbital based implementation of ADC(2)-x: Perspectives and challenges for response methods for singly and doubly excited states in large molecules. *Comput. Theor. Chem.* 1040-1041; 35–44 (2014).
17. B. Helmich; M. Sierka; J. Döbler; J. Sauer. Structure and properties of bimetallic titanium and vanadium oxide clusters. *Phys. Chem. Chem. Phys.* 16, 8441–8447 (2014).

18. G. Schmitz; B. Helmich; C. Hättig. A  $O(N^3)$  scaling PNO-MP2 method using a hybrid OSV-PNO approach with an iterative direct generation of OSVs. *Mol. Phys.* 111, 2463–2476 (2013).
19. B. Helmich; C. Hättig. A pair natural orbital implementation of the coupled cluster model CC2 for excitation energies. *J. Chem. Phys.* 139, 084114 (2013).
20. C. Hättig; D. P. Tew; B. Helmich. Local explicitly correlated second- and third-order Møller-Plesset perturbation theory with pair natural orbitals. *J. Chem. Phys.* 136, 204105 (2012).
21. B. Helmich; M. Sierka. Similarity recognition of molecular structures by optimal atomic matching and rotational superposition. *J. Comp. Chem.* 33, 134–140 (2012).
22. B. Helmich; C. Hättig. Local pair natural orbitals for excited states. *J. Chem. Phys.* 135, 214106 (2011).
23. D. P. Tew; B. Helmich; C. Hättig. Local explicitly correlated second-order Møller-Plesset perturbation theory with pair natural orbitals. *J. Chem. Phys.* 135, 074107 (2011)