Publikationsliste Helmich-Paris, Stand: 22.06.2022

1. B. Helmich-Paris; A trust-region augmented Hessian implementation for state-specific and state-averaged CASSCF wave functions. J. Chem. Phys., 156 (20), 204104 (2022)
2. B. Helmich-Paris, B. de Souza, F. Neese, and R. Izsák; An improved chain of spheres for exchange algorithm, J. Chem. Phys. 155 (10), 104109 (2021)
3. 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)
4. B. Helmich-Paris; Simulating X-ray absorption spectra with CASSCF linear response methods Int. J. Quantum Chem., e26559 (2020).
5. T. Saue et al.; The DIRAC code for relativistic molecular calculations. J. Chem. Phys. 152 (20), 204104 (2020).
6. 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).
7. B. Helmich-Paris; Benchmarks for Electronically Excited States with CASSCF Methods. J. Chem. Theory Comput., 15, 4170-4179 (2019).
8. B. Helmich-Paris; CASSCF linear response calculations for large open-shell molecules. J. Chem. Phys. 150 (17), 174121 (2019).
9. 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).
10. B. Helmich-Paris; M. Repisky; L. Visscher. Relativistic Cholesky-decomposed density matrix MP2 for large molecules. Chem. Phys. 518, 38-46 (2019).
11. 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).
12. 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).
13. 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).
14. 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).
15. 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).
16. 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).
17. B. Helmich. Paarspezifische natürliche Orbitale zur effizienten Berechnung von Coupled-Cluster-Anregungsenergien. Ph.D. thesis, Ruhr-Universität Bochum, (2014).
18. 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).

19. 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).
20. 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).
21. B. Helmich; C. Hättig. A pair natural orbital implementation of the coupled cluster model CC2 for excitation energies. J. Chem. Phys. 139, 084114 (2013).
22. 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).
23. B. Helmich; M. Sierka. Similarity recognition of molecular structures by optimal atomic matching and rotational superposition. J. Comp. Chem. 33, 134–140 (2012).
24. B. Helmich; C. Hättig. Local pair natural orbitals for excited states. J. Chem. Phys. 135, 214106 (2011).
25. 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)