Oskar Weser

Chemistry

2024 – **Postdoc**, *Massachusetts Institute of Technology*
- Group of Troy van Voorhis. Further development of quantum embedding methods. Start date 2024-09-15.

2024 **Postdoc**, *Max Planck Institute for Solid State Research*
- Group of Ali Alavi. Continued work on stochastic CI methods after defense.

2019 – 2024 **PhD**, *Max Planck Institute for Solid State Research*
- Group of Ali Alavi. Supervised by Giovanni Li Manni. Thesis title: "Novel Stochastic Methods in Electronic Structure Theory and Their Application". Defended 2024-04-10 with distinction ("summa cum laude").
- Eleven publications during PhD

2015 – 2018 **Master**, *Georg-August-Universität*, Göttingen, Final grade (German grades: 1 is best, 5 is worst) 1.3
- Thesis title: An efficient and general library for the definition and use of internal coordinates in large molecular systems
- Four publications in the course of master studies

2015 – 2016 **ERASMUS+ exchange with Sweden**, *Lund University*, Lund
- Research internship in the group of Valera Veryazov

2012 – 2017 **Scholarship of "Stiftung der deutschen Wirtschaft"**

2011 – 2015 **Bachelor**, *Georg-August-Universität*, Göttingen, Final grade 1.6
- Thesis title: Highly accurate computation of spectroscopic properties for small molecular cations

Mathematics

2012 – 2021 **Bachelor**, *Fernuniversität Hagen*, Hagen, Final grade 1.8
- Thesis title: The Dirac-Operator on Quantumgraphs

Personal details

Born, 23.Oktober 1993 (Neustadt a.d. Weinstraße)

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Publications

First authored

(1) **Weser, O.**; Alavi, A.; Manni, G. L. *Exploiting Locality in Full Configuration Interaction Quantum Monte Carlo for Fast Excitation Generation*. J. Chem. Theory Comput. **2023**, *19*, 9118–9135

(2) **Weser, O.**; Hein-Janke, B.; Mata, R. A. *Automated Handling of Complex Chemical Structures in Z-matrix Coordinates—The Chemcoord Library*. J. Comput. Chem. **2023**, *44*, 710–726

(3) **Weser, O.**; Liebermann, N.; Kats, D.; Alavi, A.; Li Manni, G. *Spin Purification in Full-CI Quantum Monte Carlo via a First-Order Penalty Approach*. J. Phys. Chem. A **2022**, *126*, 2050–2060

(4) **Weser, O.**; Guther, K.; Ghanem, K.; Li Manni, G. *Stochastic Generalized Active Space Self-Consistent Field: Theory and Application*. J. Chem. Theory Comput. **2022**, *18*, 251–272

(5) **Weser, O.**; Freitag, L.; Guther, K.; Alavi, A.; Li Manni, G. *Chemical Insights into the Electronic Structure of Fe(II) Porphyrin Using FCIQMC, DMRG, and Generalized Active Spaces*. Int. J. Quantum Chem. **2021**, *121*, 26454–26467

(6) **Weser, O.**; Veryazov, V. *In Search of the Reason for the Breathing Effect of MIL53 Metal-Organic Framework: An Ab Initio Multiconfigurational Study*. Front. Chem. **2017**, *5*, 111–119

Co-authored

(7) Li Manni, G.; Fdez. Galván, I.; [...]; **Weser, O.**; [...]; Lindh, R. *The OpenMolcas Web: A Community-Driven Approach to Advancing Computational Chemistry*. J. Chem. Theory Comput. **2023**, *19*, 6933–6991

(8) Kurz, H.; Hörner, G.; **Weser, O.**; Li Manni, G.; Weber, B. *Quenched Lewis Acidity: Studies on the Medium Dependent Fluorescence of Zinc(II) Complexes*. Chem. – Eur. J. **2021**, *27*, 15159–15171

(9) Dobrautz, W.; **Weser, O.**; Bogdanov, N. A.; Alavi, A.; Li Manni, G. *Spin-Pure Stochastic-CASSCF via GUGA-FCIQMC Applied to Iron–Sulfur Clusters*. J. Chem. Theory Comput. **2021**, *17*, 5684–5703

(10) Guther, K.; Anderson, R. J.; [...]; **Weser, O.**; Booth, G. H.; Alavi, A. *NECI: N-Electron Configuration Interaction with an Emphasis on State-of-the-Art Stochastic Methods*. J. Chem. Phys. **2020**, *153*, 34107–34131

(11) Katukuri, V. M.; Bogdanov, N. A.; **Weser, O.**; van den Brink, J.; Alavi, A. *Electronic Correlations and Magnetic Interactions in Infinite-Layer $NdNiO_2$*. Phys. Rev. B **2020**, *102*, 241112–241118

(12) Fdez. Galván, I.; Vacher, M.; [...]; **Weser, O.**; [...]; Lindh, R. *OpenMolcas: From Source Code to Insight*. J. Chem. Theory Comput. **2019**, *15*, 5925–5964

(13) Schröder, B.; Sebald, P.; Stein, C.; **Weser, O.**; Botschwina, P. *Challenging High-Level Ab Initio Rovibrational Spectroscopy: The Nitrous Oxide Molecule*. Z. Für Phys Chem. **2015**, *229*, 1663–1690

(14) Schröder, B.; **Weser, O.**; Sebald, P.; Botschwina, P. *Theoretical Rovibrational Spectroscopy beyond Fc-CCSD(T): The Cation CNC^+*. Mol. Phys. **2015**, *113*, 1914–1923

(15) Stein, C.; **Weser, O.**; Schröder, B.; Botschwina, P. *High-Level Theoretical Spectroscopic Parameters for Three Ions of Astrochemical Interest*. Mol. Phys. **2015**, *113*, 2169–2178

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