

Benedikt M. Flöser

Dr. rer. nat.

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* September 1989

Work Experience

- 05/2020–
current **Postdoc**, *Max-Planck-Institute for Chemical Energy Conversion*, Mülheim a.d. Ruhr,
Working Group: Serena DeBeer.
- Quantum chemical studies of geometric/electronic structure, and properties of enzymatic systems and model systems thereof
 - Cooperative planning of theoretical and experimental studies
 - Coordination, exchange and discussion with international collaborators of different fields
 - Participation in intra- and interinstitutional symposiums and presentation of results
- 10/2014–
04/2020 **Graduate Student**, *Christian-Albrechts-Universität*, Kiel, Working Group: Felix Tuczek.
- Synthesis and spectroscopic characterization of ligands and transition metal complexes.
 - Quantum chemical studies of geometric and electronic structure, calculation of spectra, comparison with experimental results.
 - Organization and execution of interdisciplinary cooperations with internal and external institutes.
 - Writing and publishing articles for scientific journals, solo and in collaboration.
 - Instruction of coworkers in conducting quantum chemical calculations.
 - Organization and supervision of practical lab courses for students.

Education

- 10/2014–
04/2020 **Dissertation (Dr. rer. nat.): Chemistry**, *Christian-Albrechts-Universität*, Kiel, Supervisor: Felix Tuczek, Title: Quantum Chemical Investigation of Functional Molecules.
Grade: *Magna cum laude*
- 10/2012–
09/2014 **Master of Science (M.Sc.): Chemistry**, *Christian-Albrechts-Universität*, Kiel, Focus: Inorganic and Quantum Chemistry.
Grade: 1.6
- 10/2009–
09/2012 **Bachelor of Science (B.Sc.): Chemistry**, *Christian-Albrechts-Universität*, Kiel, Focus: Inorganic Chemistry.
Grade: 1.8
- 06/2009 **Abitur**, *Hansa Gymnasium*, Hamburg.
Grade: 1.6

Languages and Software Skills

German	Native
English	Fluent
French	Basic
Elvish	Basic
Computational Chemistry	ORCA, Gaussian, Turbomole, MOPAC, MRCC, Molpro, Psi4, Molcas, Amber
Programming	Rust, Python, git, bash
Office	L ^A T _E X, LibreOffice, Microsoft Office

Trainings and Additional Experiences

- 01/2019 **Training: Teamwork & Leadership in academia**, *Christian-Albrechts-Universität*, Kiel, Dr. Jaqueline von Saldern.
- 12/2016 **Training: Project- & Time Management in Science**, *Christian-Albrechts-Universität*, Kiel, Dr. Simon Golin.
- 09/2016–
04/2018 **Leading of local church group**, *Freie evangelische Gemeinde*, Kiel, Germany.

Conference Contributions

- 09/2018 **ORCA User Meeting**, *Max-Planck-Institut für Kohlenforschung*, Mülheim a.d. Ruhr, Germany.
Poster
- 09/2017 **Norddeutsches Doktorandenkolloquium**, *Christian-Albrechts-Universität*, Kiel, Germany.
Presentation
- 08/2017 **11th Triennial Congress of the World Association of Theoretical and Computational Chemists**, Munich, Germany.
Poster
- 06/2017 **Gordon Research Conference + Seminar: Artificial Molecular Switches and Motors**, *Holderness School*, Holderness, NH, USA.
Poster, Full travel stipend
- 09/2015 **Summer School: Methods in Molecular Energy Research – Theory and Spectroscopy**, *Max-Planck-Institut für Chemische Energiekonversion*, Gelsenkirchen, Germany.
Poster
- 12/2014 **SFB 677 Winter Meeting**, *Christian-Albrechts-Universität*, Kiel, Germany.
Presentation

Publications

- 03/2020 **B. M. Flöser**, Y. Guo, C. Riplinger, F. Tuczek, F. Neese, “Detailed Pair Natural Orbital-based Coupled Cluster Studies of Spin Crossover Energetics”, *J. Chem. Theory Comput.* **2020**, *16*, 2224–2235. DOI: 10.1021/acs.jctc.9b01109
- 05/2019 T. R. Rusch, A. Schlimm, N. Krekieleh, **B. M. Flöser**, F. Röhricht, M. Hammerich, I. Lautenschläger, T. Strunskus, R. Herges, F. Tuczek, O. Magnussen, “Ordered Adlayers of a Combined Lateral Switch and Rotor”, *J. Phys. Chem. C* **2019**, *123*, 13720–13730. DOI: 10.1021/acs.jpcc.9b02469
- 04/2019 B. Herzigkeit, R. Jurgeleit, **B. M. Flöser**, N. E. Meißner, T. A. Engesser, C. Näther, F. Tuczek “Employing linear tridentate ligands with pyrazole endgroups in catalytic tyrosinase model chemistry: Does hemilability matter?”, *Eur. J. Inorg. Chem.* **2019**, 2258–2266. DOI: 10.1002/ejic.201900242
- 12/2018 B. Herzigkeit, **B. M. Flöser**, N. E. Meißner, T. A. Engesser, F. Tuczek “Click. Coordinate. Catalyze. Using CuAAC Click Ligands in Small-Molecule Model Chemistry of Tyrosinase”, *ChemCatChem* **2018**, *10*, 5402–5405. DOI: 10.1002/cctc.201801606

- 07/2018 A. Schlimm, N. Stucke, **B. M. Flöser**, T. Rusch, J. Krahmer, C. Näther, T. Strunskus, O. M. Magnussen, F. Tuczek, "Influence of a Metallic Substrate on the Small Molecule Activation Mediated by a Surface Adsorbed Complex", *Chem. Eur. J.* **2018**, *24*, 1-14. DOI: 10.1002/chem.201800911
- 04/2018 B. Herzigkeit, **B. M. Flöser**, T. A. Engesser, C. Näther, F. Tuczek, "Tyrosinase model systems supported by pyrazolylmethylpyridine ligands: electronic and steric factors influencing the catalytic activity and impact of complex equilibria in solution", *Eur. J. Inorg. Chem.* **2018**, *26*, 3058-3069. DOI: 10.1002/ejic.201800319
- 03/2018 S. Rohlf, M. Gruber, **B. Flöser**, J. Grunwald, S. Jarausch, F. Diekmann, M. Kalläne, T. Jasper-Tönnies, A. Buchholz, W. Plass, R. Berndt, F. Tuczek, K. Rossnagel, "Light-Induced Spin Crossover in an Fe(II) Low-Spin Complex Enabled by Surface Adsorption", *J. Phys. Chem. Lett.* **2018**, *9*, 1491-1496. DOI: 10.1021/acs.jpclett.8b00338
- 03/2018 N. Stucke, **B. M. Flöser**, T. Weyrich, F. Tuczek, "Nitrogen Fixation Catalyzed by Transition Metal Complexes: Recent Developments", *Eur. J. Inorg. Chem.* **2018**, 1337-1355. DOI: 10.1002/ejic.201701326
- 02/2018 H. Brandenburg, J. Krahmer, K. Fischer, B. Schwager, **B. Flöser**, C. Näther, F. Tuczek, "Coordination-Induced Spin State Switching with Nickel(II) salpn complexes: electronic vs. steric effects and influence of intermolecular interactions", *Eur. J. Inorg. Chem.* **2018**, *5*, 576-585. DOI: 10.1002/ejic.201701281
- 08/2017 **B. M. Flöser**, F. Tuczek, "Synthetic nitrogen fixation with mononuclear molybdenum complexes: electronic-structural and mechanistic insights from DFT", *Coord. Chem. Rev.* **2017**, *345*, 263-2. DOI: 10.1016/j.ccr.2016.11.003
- 08/2016 S. Hinrichsen, A.-C. Schnoor, K. Grund, **B. Flöser**, A. Schlimm, C. Näther, J. Krahmer, F. Tuczek, "Molybdenum dinitrogen complexes facially coordinated by linear tridentate PEP ligands (E = N or P): Impact of the central E donor in trans-position to N₂", *Dalton Trans.* **2016**, *45*, 14801-14813. DOI: 10.1039/C6DT02316A