

Current Position

11/2021-
today **Feodor Lynen Postdoctoral Research Fellow**, *Brown University*, Providence, RI, USA, (Advisor: Prof. C. Franklin Goldsmith)

- Automated mechanism generation for heterogeneously catalyzed reactions in particular for the production of synthetic fuels over cobalt catalyst through Fischer-Tropsch synthesis
- Quantum chemical investigation of reaction mechanism on catalysts with a special focus on developing methods for a more accurate determination of the thermophysical properties of adsorbates
- Combining automated mechanism generation and microkinetic modeling with correlated uncertainty quantification

Visit my *Introducing* profile in *Angewandte Chemie International Edition* at DOI:10.1002/anie.202311607

Research Experience

09/2021-
10/2021 **Postdoctoral Researcher**, *Karlsruhe Institute of Technology*, Karlsruhe, Germany, (Advisor: Prof. Olaf Deutschmann)

- Development of microkinetics for the exhaust gas after-treatment on Pt catalysts

08/2019-
11/2019 **Visiting Research Fellow**, *Brown University*, Providence, RI USA, (Advisor: Prof. C. Franklin Goldsmith)

- Automated mechanism generation for the CO₂ methanation on Ni catalysts with RMG
- Quantum chemistry calculations & Microkinetic modeling

11/2016-
08/2021 **Scientific Assistant/PhD Student**, *Clausthal University of Technology*, Clausthal-Zellerfeld, Germany, (Advisor: Prof. Thomas Turek)

- Experimental investigation of the transient methanation of CO₂ on Ni catalysts with kinetic measurements in a Bertly reactor and surface science methods such as temperature-programmed desorption
- Automated development of reaction mechanisms & multiscale modeling
- Preparation & characterization of heterogeneous catalysts

Industrial Experience

2013-2014 **Student employee**, *Elastica GmbH*, Osterode, Germany

- Development of rubber compounds & investigation of cross-linking kinetics
- Process development for the production of rubber molded articles

Education

2016-2021 **Doctor of Engineering (Dr.-Ing.), Chemical Engineering**, *Clausthal University of Technology*, Clausthal-Zellerfeld, Germany,
"Microkinetic Investigation of the Transient Methanation of Carbon Dioxide on Ni Catalysts"
Summa Cum Laude

2014-2016 **Master of Science, Chemical Engineering**, *Clausthal University of Technology*, Clausthal-Zellerfeld, Germany,
Thesis "Modeling and Simulation of an Alkaline Water Electrolysis"
Graduation with distinction

2011-2015 **Bachelor of Science, Chemical Engineering**, *Clausthal University of Technology*, Clausthal-Zellerfeld, Germany

Grants, Fellowships, Awards

- 2022-2024 2-year remote fellowship from the Karlsruher Institute of Technology (KIT) for a Young Investigator Group Preparation (YIG PrepPro) program
- 2022-2024 2-year Feodor Lynen Research Fellowship for postdoctoral researchers (60000€) from the Alexander von Humboldt Foundation "Unraveling the complexity of the Fischer-Tropsch synthesis on cobalt catalysts with automated reaction mechanism generation"
- 2020 Virtual research fellowship from the NaWuReT (DECHEMA/VDI)
- 2019 DAAD doctoral short-term scholarship (8000€)

Selected peer-reviewed publications

I have a total of 19 peer-reviewed publications, 11 as first author. I have 409 citations and an h-index of 10 (2023/10/07, see Google Scholar https://scholar.google.com/citations?user=yuUY1_EAAAAJ&hl=en). The impact factor of journals is reported in parentheses.

- 1.† **B. Kreitz***, P. Lott, A. J. Medford, F. Studt, O. Deutschmann, and C. F. Goldsmith. "Automated Generation of Microkinetics for Heterogeneously Catalyzed Reactions Considering Correlated Uncertainties". *Angew. Chem. Int. Ed.*, 62 (39), 2023, e202306514 (16.6)
2. **B. Kreitz***, K. Abeywardane, and C. F. Goldsmith. "Linking Experimental and Ab-initio Thermochemistry of Adsorbates with a Generalized Thermochemical Hierarchy". *J. Chem. Theory Comput.*, 19 (13), 2023, 4149–4162 (5.5)
3. **B. Kreitz***, P. Lott, K. Blöndal, J. Bae, S. Angeli, Z. W. Ulissi, F. Studt, C. F. Goldsmith, and O. Deutschmann. "Detailed microkinetics for the oxidation of exhaust gas emissions through automated mechanism generation". *ACS Catal.*, 12 (18), 2022, 11137–11151 (12.9)
4. **B. Kreitz**, G. D. Wehinger, C. F. Goldsmith, and T. Turek. "Microkinetic modeling of the transient CO₂ methanation with DFT-based uncertainties in a Berty reactor". *ChemCatChem* 2022, e202200570 (4.5)
5. S. Anderson, **B. Kreitz**, T. Turek, and G. D. Wehinger. "Assessment of concentration and temperature distribution for an exothermic reaction in a Berty reactor". *Ind. Eng. Chem. Res.*, 61 (30), 2022, 10790–10803 (4.2)
6. **B. Kreitz***, K. Sargsyan, K. Blöndal, E. J. Mazeau, R. H. West, G. D. Wehinger, T. Turek, and C. F. Goldsmith. "Quantifying the Impact of Parametric Uncertainty on Automatic Mechanism Generation for CO₂ Hydrogenation on Ni(111)". *JACS Au*, 1 (10), 2021, 1656–1673 (8.0)
7. **B. Kreitz**, G. D. Wehinger, C. F. Goldsmith, and T. Turek. "Microkinetic Modeling of the CO₂ Desorption from Supported Multifaceted Ni Catalysts". *J. Phys. Chem. C*, 125 (5), 2021, 2984–3000 (3.7)
8. **B. Kreitz***, A. Martínez Arias, J. Martin, A. P. Weber, and T. Turek. "Spray-Dried Ni Catalysts with Tailored Properties for CO₂ Methanation". *Catalysts*, 10 (12), 2020, 1410 (4.5)
9. J. Friedland, **B. Kreitz**, H. Grimm, T. Turek, and R. Güttel. "Measuring Adsorption Capacity of Supported Catalysts with a Novel Quasi-Continuous Pulse Chemisorption Method". *ChemCatChem*, (12), 2020, 1–15 (4.5)
10. G. D. Wehinger, **B. Kreitz**, A. Nagy, and T. Turek. "Characterization of a modular Temkin reactor with experiments and computational fluid dynamics simulations". *Chem. Eng. J.*, 389 2020, 124342 (15.1)
11. **B. Kreitz***, G. D. Wehinger, and T. Turek. "Dynamic simulation of the CO₂ methanation in a micro-structured fixed-bed reactor". *Chem. Eng. Sci.*, 195 2019, 541–552 (4.7)
12. P. Haug, **B. Kreitz**, M. Koj, and T. Turek. "Process modelling of an alkaline water electrolyzer". *Int. J. Hydrogen Energy*, 42 (24), 2017, 15689–15707 (7.2)

† Rated as Very Important Paper

* Corresponding author

Selected talks at conferences

I have given 20 talks at national and international conferences. Additionally, I was invited as a seminar speaker in numerous department such as in the theory groups of BASF SE and University of Stuttgart.

1. "Tackling the Complexity of Fischer-Tropsch Synthesis with Automated Mechanism Generation", *ACS Fall (invited)*, 2023, San Francisco, USA
2. "Microkinetic Modeling with Accurately Predicted Pathways Involving Bidentate Adsorbates: An Ethane Hydrogenolysis Study with RMG", *28 North American Catalysis Society Meeting*, 2023, Providence, USA
3. "Uncertainty Quantification in Automated Mechanism Development for Heterogeneously Catalyzed Reactions", *ACS Spring (invited)*, 2023, Indianapolis, USA
4. "Coupling Experimental and Ab-initio Thermochemistry of Adsorbates in a Generalized Thermochemical Hierarchy", *56th German Catalysis Meeting*, 2023, Weimar, Germany
5. "Microkinetic Investigation of the Transient CO₂ Methanation on Ni Catalysts in a Berty Reactor", *AIChE Meeting*, 2022, Phoenix, USA
6. "Automated generation of mechanisms for complex reaction mixtures in emission control catalysis", *ACS Fall*, 2022, Chicago, USA
7. "Automated Discovery of Reaction Mechanisms Considering DFT-Based Uncertainties", *27 North American Catalysis Society Meeting*, 2022, New York City, USA
8. "Dynamic methanation of CO₂ - Effects of concentration forcing", *Annual Meeting on Reaction Engineering*, 2018, Würzburg, Germany

Teaching & Mentoring Experience

- Guest lecturer & teaching assistant *ENGN2770: Atomistic Reaction Engineering* at Brown University with Prof. Andrew A. Peterson during fall semester '22
- Teaching assistant & guest lecturer for *Chemical Reaction Engineering* and *Computer Aided Design of Chemical Reactors* at Clausthal University of Technology
- Organization of open-source software ("RMG") workshops at the 2022 & 2023 ACS Fall Meetings
- Supervision & mentoring of 3 Master & 3 Bachelor students, 2 group projects, 1 international exchange student

Community Engagement

- Review service for *Proceedings of the Combustion Institute*, *International Journal of Hydrogen Energy*, *Chemical Engineering Journal*, *Journal of Catalysis*, *Computer Physics Communication*, *ACS Omega*
- Lead author of the annual chemical engineering report for the German Chemical Society (GDCh) "Trends in Chemical Technology 2022" (see DOI: 10.1002/nadc.20224124649)
- Contribution to the remote international workshop "Quo vadis in multiscale modeling?-A perspective" (see DOI: 10.1016/j.cherd.2022.05.030)
- Committee member of the NaWuReT (German Early Career Reaction Engineers, DECHEMA) since 2020
 - Organization of summer schools, colloquia, and lecture series (see e.g. DOI: 10.1002/cite.202100200) to foster the exchange of chemistry and chemical engineering students in Germany
- Member of the DOE Basic Energy Sciences (BES) Early Career Network planning committee since 2023