Dr. Jonny Proppe

Position	Tenure-Track Assistant Professor since 10/2021
Affiliation	TU Braunschweig Institute of Physical and Theoretical Chemistry Gauss Str 17, 38106 Braunschweig, Germany
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Scientific Research

Mission	Development and application of data-driven methods to understand and efficiently predict reactions and (bio)physical properties of molecules, with a focus on CO_2 and drugs.
Methods	Machine learning; uncertainty quantification; cheminformatics; quantum chemistry.

Academic Qualifications

2018 – 2021	Postdoctoral research at **Harvard University**, United States; **University of Toronto**, Canada; **University of Göttingen**, Germany.
2014 – 2018	Doctoral studies (Dr. sc.), **ETH Zürich**, Switzerland. Supervisor: **Markus Reiher**.
2008 – 2014	Chemistry studies (BSc, MSc), **University of Hamburg**, Germany.

Funding and Awards

2023 – 2026	DFG Project 512350771: "Towards chemical space exploration for functional nanostructured systems" (collaboration with Prof. Carmen Herrmann).
2020	*IBM Research* prize for the best dissertation of the year in the computational sciences.
2018 – 2019	*Early Postdoc.Mobility* fellowship by the SNSF for postdoctoral stays at Harvard University and the University of Toronto (with **Alán Aspuru-Guzik**).

Representative Publications

1. Unveiling CO_2 reactivity with Data-Driven Methods
M. Eckhoff, K. L. Bublitz, J. Proppe, *Digit. Discov.* **2025**, *4*, 868, https://doi.org/10.1039/d5dd00020c

2. Predicting and Explaining Yields with Machine Learning for Carboxylated Azoles and Beyond
K. Janssen, J. Proppe, *J. Chem. Inf. Model.* **2025**, *65*, 1862, https://doi.org/10.1021/acs.jcim.4c02336

3. Relevance and Potential Applications of C2-Carboxylated 1,3-Azoles
K. Janssen, J. Kirchmair, J. Proppe, *ChemMedChem* **2024**, *19*, e202400307, https://doi.org/10.1002/cmdc.202400307

4. Quantitative Structure–Reactivity Relationships for Synthesis Planning – The Benzhydrylium Case
M. Eckhoff, J. V. Diedrich, M. Mücke, J. Proppe, *J. Phys. Chem. A* **2024**, *128*, 343, https://doi.org/10.1021/acs.jpca.3c07289

5. The Computational Road to Reactivity Scales
M. Vahl, J. Proppe, *Phys. Chem. Chem. Phys.* **2023**, *25*, 2717, https://doi.org/10.1039/d2cp03937k