Prof. Dr. Johannes T. Margraf

University of Bayreuth
Physical Chemistry V: Theory and Machine Learning
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Academic Positions

University of Bayreuth / Professor of Physical Chemistry
SEPTEMBER 2023 - PRESENT, BAYREUTH

Fritz-Haber-Institute / Research Group Leader
FEBRUARY 2021 - AUGUST 2023, BERLIN

Technical University Munich / PostDoc and Group Leader
APRIL 2017 - JANUARY 2021, MUNICH

University of Florida / PostDoc
MARCH 2016 -MARCH 2017, GAINESVILLE

Education

PhD / FAU Erlangen-Nürnberg (summa cum laude)

Physical and Computational Chemistry (2015)

M.Sc. / FAU Erlangen-Nürnberg

Molecular Science (2012)

B.Sc. / FAU Erlangen-Nürnberg

Molecular Science (2010)

Supervision and Mentoring

(Co-)supervision of 6 completed and 6 ongoing doctorates, as well as 5 theses (B.Sc. and M.Sc.). Mentoring of 7 PostDocs. Supporting postdocs and doctoral students in obtaining scholarships, e.g. via the Alexander von Humboldt Foundation (2), the China Scholarship Council (2) and the Chemical Industry Fund (1).

Leadership Roles

(Co-)Organization of six international workshops on chemical machine learning and atomistic simulations since 2018 (e.g. funded by Psi-k and DFG). Associate Editor for *NPJ Comput. Mater.* Director of the Bayreuth *Research Center for AI in Science and Society*. Membership in the *German Chemical Society* and *German Physical Society*. Scholar of the *European Laboratory for Learning and Intelligent Systems* (ELLIS).

Conference Presentations

39 invited talks and department seminars (e.g. at Cambridge, Korean Advanced Institute of Science and Technology, University of Luxembourg, Telluride Worksop USA, TU Vienna, etc.).

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Teaching Experience

M.Sc. level courses on *Solid State Theory* and *Advanced Electronic Structure Theory*, B.Sc. level courses on *Introductory Quantum Mechanics* and *Scientific Programming* at TU Munich. M.Sc. level course on *Chemical Machine Learning* at Uni Potsdam. Various courses on *Physical Chemistry*, *Quantum Chemistry* and *Data Science in Chemistry* at Uni Bayreuth.

Selected Publications

(1) Jakob, K. S.; Walsh, A.; Reuter, K.; **Margraf, J. T.**
Learning Crystallographic Disorder: Bridging Prediction and Experiment in Materials Discovery
Advanced Materials **2025**, e14226.

(2) Vondrák, M.; Reuter, K.; **Margraf, J. T.**
Pushing Charge Equilibration Based Machine Learning Potentials to their Limits
NPJ Comput. Mater. **2025**, 11, 288.

(3) Xu, W.; Diesen, E.; He, T.; Reuter, K.; **Margraf, J. T.**
Discovering High Entropy Alloy Electrocatalysts in Vast Composition Spaces with Multiobjective Optimization
Journal of the American Chemical Society **2024**, 146, 7698–7707.

(4) Jung, H.; Sauerland, L., Stocker, S.; Reuter, K.; **Margraf, J. T.**
Machine-Learning Driven Global Optimization of Surface Adsorbate Geometries
NPJ Computational Materials **2023**, *9*, *114*.

(5) **Margraf, J. T.**
Science-Driven Atomistic Machine Learning
Angewandte Chemie **2023**, *62*, *e202219170*.

(6) Chen, K.; Kunkel, C.; Cheng, B.; Reuter, K.; **Margraf, J. T.**
Physics-Inspired Machine Learning of Localized Intensive Properties
Chemical Science **2023**, 14, *4913-4922*.

(7) Stocker, S.; Gasteiger, J.; Becker, F.; Günnemann, S.; **Margraf, J. T.**
How Robust are Modern Graph Neural Network Potentials in Long and Hot Molecular Dynamics Simulations?
Machine Learning: Science and Technology **2022**, 3, 045010.

(8) Wengert, S.; Csányi, G.; Reuter, K.; **Margraf, J. T.**
Data-Efficient Machine Learning for Molecular Crystal Structure Prediction.
Chemical Science **2021**, *12*, 4536–4546.

(9) **Margraf, J. T.**; Reuter, K.
Pure Non-Local Machine-Learned Density Functional Theory for Electron Correlation.
Nature Communications **2021**, *12*, 344.

(10) Stocker, S.; Csányi, G.; Reuter, K.; **Margraf, J. T.**
Machine Learning in Chemical Reaction Space.
Nature Communications **2020**, *11*, 5505.

95 peer-reviewed publications, 22 as first author, 31 as corresponding author

Metrics: h-Index 41, i10-Index 74 (Google Scholar Profile, Jan 2026)

Funding and Fellowships

DFG SPP Project / Machine Learning in Chemical Engineering
2025-2028

Autoregressive Deep Learning for Accelerated Multiscale Simulation of Electrochemical Flow Reactors
(Total Sum: EUR 233.810,56 / Personal Part: EUR 233.810,56)

BMWK Project / 'KernKat'
2025-2028
Kern-Schale Katalysatorsysteme für geringe Edelmetallbeladungen, hohe Umwandlungseffizienzen und hohe Lebensdauern in der Wasserelektrolyse mit saurer Polymerelektrolytmembran
(Total Sum: EUR 4.089.129 / Personal Part: EUR 283.038,97)

BMBF Project / 'CarboDiol 2.0'
2024-2027
Von Kohlenhydraten aus sekundären Rohstoffquellen zu Chemierohstoffen
(Total Sum: EUR 2.136.098 / Personal Part: EUR 300.215)

Project Grant / 'UniSysCat' Excellenzcluster
2023-2026
Closing the gap between first principle kinetic Monte Carlo simulations to mean field meso-scale models by means of machine learning
(Total Sum: EUR 182,400 / Personal Part EUR 91,200)

IGGSE Project Grant 'CatGraph' / DFG Graduate School GSC81
2017-2020
Funding for a collaborative project with two PhD students (3 years) in chemistry and computer science.
(Total: EUR 222,600 / Personal Part: EUR 111,600)

Postdoctoral Fellowship / TUM University Foundation
2018
(Personal Grant: EUR 31,800)

Return Fellowship / Alexander-von-Humboldt-Foundation
2017
(Personal Grant: EUR 36,000)

Feodor-Lynen-Fellowship / Alexander-von-Humboldt-Foundation
2016
(Personal Grant: EUR 42,636)

Beilstein PhD Scholarship / Beilstein Foundation
2012-2015
(Personal Grant: EUR 59,400)