

PERSONAL INFORMATION **Jannik Philipp Roth**

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🌐 <https://github.com/jannik-roth>

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Date of birth 21 February 1997 | Nationality German

EDUCATION

- 05/2023 – today **Doctoral Candidate Chemistry**
at the *University of Bonn* in Bonn, Germany
Working Title: Uncertainty Quantification in Machine Learning applied to Cheminformatics
Supervisor: Prof. Dr. T. Bredow and Prof. Dr. J. Hasenauer
- 10/2020 – 12/2022 **Master of Science Chemistry**
at the *Ludwig Maximilian University of Munich* in Munich, Germany
MSc Thesis Supervisor: Prof. Dr. C. Ochsenfeld
overall grade: very good (1.0)
- 10/2019 – 09/2020 **Research Stay**
at the *Università degli Studi di Milano-Bicocca* in Milan, Italy
Dipartimento di Scienza dei Materiali, Quantum Chemistry Lab
Supervisor: Prof. Dr. G. Pacchioni
- 10/2016 – 09/2019 **Bachelor of Science Chemistry**
at the *University of Bonn* in Bonn, Germany
BSc Thesis Supervisor: Prof. Dr. T. Bredow
overall grade: excellent (1.2)

TECHNICAL SKILLS

- Programming Languages** Python (advanced), C++ (beginner), Fortran (beginner)
- Cheminformatics** RDKit (advanced)
- Data Processing, Analysis, and Visualization** SciPy (advanced), NumPy (advanced), scikit-learn (advanced), pandas (intermediate), matplotlib (advanced), seaborn (advanced)
- Deep Learning** PyTorch (advanced), PyTorch Lightning (intermediate), Weights & Biases (intermediate)
- Scientific Computing** familiar with the Linux operating system, experience in high-performance computing environment

PUBLICATIONS

- [1] **Jannik P. Roth** and Jürgen Bajorath. “Unraveling learning characteristics of transformer models for molecular design”. In: *Patterns* 6.12 (2025). doi: 10.1016/j.patter.2025.101392.
- [2] **Jannik P. Roth** and Jürgen Bajorath. “Protocol to calculate and compare exact Shapley values for different kernels in support vector machine models using binary features”. In: *STAR Protocols* 5.4 (2024). doi: 10.1016/j.xpro.2024.103450.
- [3] **Jannik P. Roth** and Jürgen Bajorath. “Machine learning models with distinct Shapley value explanations decouple feature attribution and interpretation for chemical compound predictions”. In: *Cell Reports Physical Science* 5.8 (2024). doi: 10.1016/j.xcrp.2024.102110.
- [4] **Jannik P. Roth** and Jürgen Bajorath. “Relationship Between Prediction Accuracy and Uncertainty in Compound Potency Prediction Using Deep Neural Networks and Control Models”. In: *Scientific Reports* 14.1 (2024). doi: 10.1038/s41598-024-57135-6.
- [5] Xiaojuan Yu, **Jannik P. Roth**, Junjun Wang, Eric Sauter, Alexei Nefedov, Stefan Heißler, Gianfranco Pacchioni, Yuemin Wang, and Christof Wöll. “Chemical Reactivity of Supported ZnO Clusters: Undercoordinated Zinc and Oxygen Atoms as Active Sites”. In: *ChemPhysChem* 21.23 (2020). doi: 10.1002/cphc.202000747.
- [6] **Jannik P. Roth** and Gianfranco Pacchioni. “Influence of Strain on Acid–Basic Properties of Oxide Surfaces”. In: *The Journal of Physical Chemistry C* 124.35 (2020). doi: 10.1021/acs.jpcc.0c05913.
- [7] Leander Haug, **Jannik P. Roth**, Marco Thaler, Dominik Steiner, Alexander Menzel, Sergio Tosoni, Gianfranco Pacchioni, and Erminald Bertel. “Precursor chemistry of h-BN: adsorption, desorption, and decomposition of borazine on Pt(110)”. In: *Physical Chemistry Chemical Physics* 22.20 (2020). doi: 10.1039/D0CP00112K.

Underlined authors are joint first authors with equal contribution.

AWARDS AND ACHIEVEMENTS

- 05/2024 – today Doctoral Scholarship
German Academic Scholarship Foundation (Studienstiftung des deutschen Volkes)
- 12/2022 MSc Thesis Prize
Römer-Preis 2023 of the Römer-Stiftung for excellent scientific achievements in chemistry
- 04/2018 – 12/2022 BSc/MSc Scholarship
German Academic Scholarship Foundation (Studienstiftung des deutschen Volkes)

TEACHING EXPERIENCE

- 03/2026 – today Undergraduate courses and lab rotations in theoretical chemistry (University of Bonn)
- 05/2023 – 11/2025 Graduate course “Molecular Modeling and Drug Design” (University of Bonn)
- 10/2017 – 09/2019 Undergraduate courses (University of Bonn):
- Physical Chemistry I: Thermodynamics, Kinetics, Electrochemistry
 - Physical Chemistry II: Statistical Thermodynamics
 - Lab Course Qualitative Analysis
 - Preliminary Courses
 - Theoretical Chemistry II: Group Theory