

Anton Zamyatin

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Austrian/EU citizen

Research Interests: Deep Learning for Chemistry · Uncertainty Quantification

SKILLS

Programming Python, C/C++, Java

Deep Learning PyTorch, Lightning

Software Eng. Docker, Git, Spring Boot, Angular, React, Vue, SQL

Languages English (IELTS 8), German (native), Russian (fluent), French (basic)

EXPERIENCE

TU Wien, Heid Lab · Research Assistant

Apr 2025 – present

- Researching deep learning methods for predicting chemical reaction activation energies.
- Lead developer of ChemTorch (modular framework for reaction deep learning; [code](#) / [preprint](#)).

Google Developer Group @TU Wien · Co-Organizer

Mar 2025 – present

- Austria's largest chapter of Google's global developer network, based in Vienna.
- Organize tech talks, workshops, and paper discussions for 30–60 participants.

Essen auf Rädern (Student Software Project) · Software Engineer

Mar 2024 – Jun 2024

- Developed order management software for a social service SME which delivers meals to the elderly.
- Full-stack development using Java, Spring Boot, & Angular.

Max Perutz Labs, Kovarik Lab · Summer Intern

Jul 2023 – Sep 2023

- Evaluated gene expression techniques for a synthetic protein construct for inflammation research.
- Conducted transfection and transduction experiments in human cell lines.
- Performed protein expression assays (Western Blot, qRT-PCR, ELISA, IF microscopy).

EDUCATION

TU Wien · MSc Computational Science and Engineering

Oct 2025 – present

- Mathematics (functional analysis, PDEs), Numerics, HPC.
- Specialization: Theoretical and Computational Chemistry.

TU Wien · BSc Computer Science, GPA 1.38

Oct 2022 – Jul 2025

- Thesis on "Efficient Ensembling for Uncertainty Quantification of Neural Networks"
- Focus: Deep Learning + Software Engineering

University of Vienna · Molecular Biology

Oct 2022 – Jun 2024

- Completed 50 credits alongside computer science degree.
- Focus: Chemistry + Structural Biology.

Theresianische Akademie Wien · High School, GPA 1.0

Sep 2014 – Jun 2022

PUBLICATIONS

- A. Zamyatin, P. Indri, S. Malhotra, T. Gärtner, **Is BatchEnsemble a Single Model? On Calibration and Diversity of Efficient Ensembles**, EIML@EurIPS 2025 Workshop
- J. De Landsheere*, A. Zamyatin*, J. Karwounopoulos, E. Heid, **ChemTorch: A Deep Learning Framework for Benchmarking and Developing Chemical Reaction Property Prediction Models** (*equal contribution)

PERSONAL PROJECTS

quizard LLM-powered flashcard generator with Python, React and Docker ([code](#))

message-broker DNS-based message broker with leader election and UDP monitoring in Java ([code](#))

cdc-covid-19 Comorbidity analytics dashboard Python and Streamlit ([code](#))