

# Anton Zamyatin

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Austrian/EU citizen

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*Research Interests: Deep Learning for Chemistry · Uncertainty Quantification*

## SKILLS

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**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

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**TU Wien, Heid Lab** · *Machine Learning Engineer*

Apr 2025 – present

- Researching deep learning models for chemical reactions and reaction property prediction.
- Lead developer of ChemTorch (modular framework for reaction 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

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**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

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- 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

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**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](#))