

# KRZYSZTOF MAZIARZ

✉ [krzysztof.s.maziarz@gmail.com](mailto:krzysztof.s.maziarz@gmail.com)

🔗 [scholar.google.pl/citations?user=BA8bBVkAAAAJ](https://scholar.google.pl/citations?user=BA8bBVkAAAAJ)

🐦 @maziarzkris

📍 London, UK

## WORK EXPERIENCE

Microsoft Research, AI for Science

**Principal Researcher**

📅 10/24 – Now (10 months)

**Senior Researcher**

📅 02/20 – 10/24 (5 years) 📍 Cambridge, UK

Led the development of generative models of molecules (used at Novartis, 150+ drug proposals synthesized), reaction prediction models, and planning algorithms for retrosynthesis; contributed to work on few-shot molecular property prediction and MCMC for solving Schrödinger equation. Worked with GNNs, Transformers, LLMs, autoencoders, neurosymbolic models, search (A\*, AlphaGo-style MCTS), meta-learning, diffusion, RL. 4 main track publications at NeurIPS, ICLR, ICML.

Google Brain / Google AI

**Software Engineering Intern x3**

📅 07/19 – 09/19 (3 months) 📍 Zurich, Switzerland

📅 07/18 – 10/18 (3 months) 📍 Zurich, Switzerland

📅 07/16 – 09/16 (3 months) 📍 Mountain View, US

Researched multi-task learning (published at ICLR-W); Neural Architecture Search by combining RL + evolution (ICML-W, deployed in Google AutoML); and Mixture-of-Experts models for machine translation (ICLR, the pioneering MoE work, 60B+ parameter models in 2016).

Tensorflight

**Research Intern**

📅 11/18 – 04/19 (6 months) 📍 Warsaw, Poland

Worked on multi-modal fusion on street-view image data; applied to building analysis; published at AAAI.

Jane Street Capital

**Developer Intern**

📅 07/17 – 09/17 (3 months) 📍 London, UK

Wrote software in OCaml; built a framework for testing trading systems and a low-level caching library.

## EDUCATION

Ph.D., Computer Science

Pending; based on work published during my time at MSR

**Freie Universität Berlin**

Bachelor's & Master's, Computer Science

**Jagiellonian University in Kraków**

## SELECTED PUBLICATIONS

- [Maziarz](#), Liu, Misztela, Tripp, Li, Kornev, (...), Segler "Chemist-aligned retrosynthesis by ensembling diverse inductive bias models", preprint
- [Maziarz](#), Tripp, Liu, Stanley, Xie, Gaiński, Seidl, Segler "Re-evaluating Retrosynthesis Algorithms with Synthesus", **Faraday Discussions 2024**
- Tripp, [Maziarz](#), Lewis, Segler, Hernández-Lobato *Retro-fallback: Retrosynthetic Planning in an Uncertain World*, **ICLR 2024**
- Liu, Xue, Xie, Xia, Tripp, [Maziarz](#), Segler, (...), Liu "Retrosynthetic Planning with Dual Value Networks", **ICML 2023**
- [Maziarz](#), Jackson-Flux, (...), Segler, Brockschmidt "Learning to Extend Molecular Scaffolds with Structural Motifs", **ICLR 2022**
- Stanley, Bronskill, [Maziarz](#), (...), Brockschmidt "FS-Mol: A Few-Shot Learning Dataset of Molecules", **NeurIPS 2021**
- Shazeer, Mirhoseini, [Maziarz](#), Davis, Le, Hinton, Dean "Outrageously large neural networks: The sparsely-gated mixture-of-experts layer", **ICLR 2017**

## OPEN-SOURCE CODE

[github.com/microsoft/syntheseus](https://github.com/microsoft/syntheseus) ★ 160

Package for combining reaction prediction models with planning algorithms in a plug-and-play manner; backbone for retrosynthesis efforts at MSR AI for Science.

[github.com/microsoft/molecule-generation](https://github.com/microsoft/molecule-generation) ★ 305

Inference code for a GNN-based autoregressive generative model of molecular graphs; since 2021 used internally by Novartis in several drug design projects.

## SELECTED ACHIEVEMENTS

- 14th and 34th place in **ACM ICPC Finals** (2016, 2017)
- Finalist of **Facebook HackerCup** (2016; 25 finalists)
- Advanced to the finals of Distributed **Google Code Jam** (2018; 20 finalists)
- **Area Chair** for NeurIPS (2024, 2025), ICML (2024)
- **Reviewer** for ICLR, ICML, NeurIPS, TMLR (2020+, including 4 "best reviewer" awards)
- 10th place in finals of **Google HashCode** (2018)
- Rated "red" (top 0.2%) by several major competitive programming sites (Codeforces, TopCoder)
- Creator of programming problems for ACM ICPC regionals and International Olympiad in Informatics
- First Prize in Putnam Mathematical Competition mirror (2016, 2018)