

Arthur Kosmala

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Experience

09/2025 – 01/2026 /
04/2026 – 07/2026
(part-time extension)

PhD Research Intern • Meta FAIR Chemistry Team, San Francisco

- Derived & built a novel parallelism method (speculative sampling) for 3-9x faster molecular dynamics
- Accepted at ICML 2026. Internship extension granted to finalize and integrate the work with the team

09/2023 – now

PhD Student • Data Analytics and Machine Learning Group, Technical University of Munich

- Research profile: physics-informed machine learning for graphs and molecules
- Three accepted first-author conference papers by now

12/2022 – 06/2023

Research Assistant • Theory Division, Max Planck Institute for the Science of Light, Erlangen

- Topic: flow-based generative models for multiscale sampling of lattice spin configurations
- Proved an optimal-transport-based correspondence to field-theoretic coarse-graining tools

11/2021 – 03/2023
(part-time)

Quantum Computing Intern • E.ON Digital Technology, Munich

- Studied the effect of data encoding choice on unsupervised quantum anomaly detection
- Mix of analytical methods and testing on cloud quantum hardware with real and synthetic data

06/2022 – 08/2022

Flatiron Machine Learning X Science Summer School • Simons Foundation, New York City

Co-authored a NeurIPS workshop paper (learning phase-space transforms for mechanics simulation)

10/2018 – 02/2019

Student Assistant • Ultrafast Nanophotonics Group • LMU Munich

Built an educational light ray simulation for use in optics lectures with C++

Prior Education

10/2019 – 07/2023

Technical University & Ludwig Maximilian University of Munich

MSc in Theoretical and Mathematical Physics - 1.1 (1.0 is best)

MSc thesis: Ewald-based Long-Range Message Passing for Molecular Graphs

10/2019 – 07/2020

University of Oxford

*MSc in Mathematical and Theoretical Physics – **Distinction** (no numerical scale, Distinction is best)*

Focus area: Condensed Matter Physics

10/2016 – 09/2019

Ludwig Maximilian University of Munich

BSc in Physics – 1.0 (top 3%, 1.0 is best)

BSc thesis: Geometric Thermodynamics on Contact Manifolds

Selected Publications

- [1] **Kosmala, A.**, Günnemann, S., Gao, M., Wood, B. (2026). Speculative Sampling For Faster Molecular Dynamics. Accepted at **ICML 2026**. Preprint URL: arxiv.org/pdf/2606.02455
 - [2] Geisler, S.*, **Kosmala, A.***, Herbst, D., Günnemann, S. (2024). Spatio-Spectral Graph Neural Networks. **NeurIPS 2024**.
 - [3] Schuchardt, J., Stoian, M., **Kosmala, A.**, Günnemann, S. (2024). Unified Mechanism-Specific Amplification by Subsampling and Group Privacy Amplification. **NeurIPS 2024**.
 - [4] **Kosmala, A.**, Gasteiger, J., Gao, N., Günnemann, S. (2023). Ewald-based Long-Range Message Passing for Molecular Graphs. **ICML 2023**.
 - [5] Daigavane, A., **Kosmala, A.**, Cranmer, M., Smidt, T., Ho, S. (2022). Learning Integrable Dynamics with Action-Angle Networks. **NeurIPS 2022 ML4PS Workshop**.
- * **equal contribution.**

Skills

Software
Programming Courses
Languages

Python (PyTorch, Scientific Stack) • C++ • LaTeX • Git • Linux

Advanced Python Programming • Python for Physicists • C++ for Physicists (LMU Munich, ~100h)

German (native) • Polish (native) • English (CEFR C2, highest level) • Latin ('Latinum' certificate)

Awards

10/2024

Runner-up @ MDSI Best Paper of 2023, cross-faculty award for work on Ewald Message Passing

07/2024 – now

Linde / MDSI Doctoral Fellowship, funding for 50% of PhD position, data science training program

09/2023

G-Research Grant, funding for presentation of paper at ICML 2023 conference

07/2016 – 10/2022

Max Weber Scholarship, study-long education grant by the federal state of Bavaria

10/2019 – 06/2020

DAAD One-Year Grant, German Academic Exchange Service, funding for studies at Oxford