Minkyu Kim

Seoul, South Korea | minkyu-kim@kaist.ac.kr | +82-10-6342-9959
Website | GitHub | LinkedIn | Google Scholar

Summary

I am a Ph.D. student in Artificial Intelligence at KAIST (anticipated graduation 02/29), advised by Sungsoo Ahn. I received my B.S. in Mathematics from POSTECH, and I am currently a research intern at Mila, hosted by Alex Hernández-García. My research focuses on flow-based generative models and diffusion samplers, and on their application to AI for science, in particular molecular conformer generation and materials discovery.

Academic Placement and Employment

Korea Advanced Institute of Science and Technology (KAIST) — Feb 2025 – Present
Ph.D. Student, SPML Lab (Advisor: Sungsoo Ahn) — Seoul, South Korea

Mila – Quebec Artificial Intelligence Institute — Jul 2026 – Oct 2026
Research Intern (Host: Alex Hernández-García) — Montréal, QC

Publications

CatFlow: Co-generation of Slab-Adsorbate Systems via Flow Matching — ICML 2026
Minkyu Kim, Nayoung Kim, Honghui Kim, Sungsoo Ahn arXiv

On Scalable and Efficient Training of Diffusion Samplers — NeurIPS 2025
Minkyu Kim, Kiyoung Seong, Dongyeop Woo, Sungsoo Ahn, Minsu Kim arXiv

Energy-Based Generator Matching: A Neural Sampler for General State Space — NeurIPS 2025
Dongyeop Woo, Minsu Kim, ***Minkyu Kim***, Kiyoung Seong, Sungsoo Ahn arXiv

AtomMOF: All-Atom Flow Matching for MOF-Adsorbate Structure Prediction — arXiv 2026
Nayoung Kim, Honghui Kim, Sihyun Yu, ***Minkyu Kim***, Seongsu Kim, Sungsoo Ahn arXiv

Education

Korea Advanced Institute of Science and Technology (KAIST) — 02/25 – 02/29 (expected)
Ph.D. in Artificial Intelligence, advised by Prof. Sungsoo Ahn

Technische Universität Wien, Exchange Student in Applied Mathematics — Feb 2023 – Aug 2023

Pohang University of Science and Technology (POSTECH) — Feb 2020 – Feb 2024
B.S. in Mathematics

Academic Services

Reviewer

- Conference: ICLR 2026, ICML 2026, NeurIPS 2026
- Journal: TMLR

Workshop Student Committee

- AI4Science Korea Workshop, ICML 2026
- ProbML 2026

Talks

Generative Modeling for Catalyst Design — Aug 2026

- AI for materials reading group at Mila - Quebec Artificial Intelligence Institute (Montreal, Canada)

Technical Skills

Programming:	Python, C++, JAX
Libraries:	PyTorch, ASE, pymatgen, OpenMM, nvalchemi-toolkit, kUPS
Research methods:	Flow matching, Diffusion models, GFlowNets, Boltzmann generators, Stochastic interpolants, Guidance
Systems:	Linux, Git, Slurm, Kubernetes