

Minkyu Kim

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Summary

I'm a 1st-year Ph.D. candidate in at KAIST AI, advised by [Sungsoo Ahn](#). I majored in Mathematics, and recently led a project on scalable diffusion sampler for molecular conformer generation with sample-efficient training. Currently, I am developing generative models for catalyst design conditioned on adsorbates.

Publications

- CatFlow: Co-generation of Slab-Adsorbate Systems via Flow Matching** 2026
Minkyu Kim, Nayoung Kim, Honghui Kim, Sungsoo Ahn
arxiv.org/abs/2602.05372 (arXiv)
- On scalable and efficient training of diffusion samplers** 2025
Minkyu Kim, Kiyoun Seong, Dongyeop Woo, Sungsoo Ahn, Minsu Kim
arxiv.org/abs/2505.19552 (NeurIPS 2025)
- Energy-based generator matching: A neural sampler for general state space** 2025
 Dongyeop Woo, Minsu Kim, *Minkyu Kim*, Kiyoun Seong, Sungsoo Ahn
arxiv.org/abs/2505.19646 (NeurIPS 2025)

Education

- Ph.D. Korea Advanced Institute of Science and Technology (KAIST)**, Kim Jaechul Seoul, South Korea
 Graduate School of Artificial Intelligence Feb 2025 – present
 - [Structured and Probabilistic Machine Learning Lab](#) @ Sungsoo Ahn
 - Topic: Diffusion samplers, Molecular dynamics (MD), Generative Flow Networks (GFlowNet), Catalyst
- E.S. Technische Universität Wien (TU Wien)**, Applied Mathematics Vienna, Austria
 Exchange Student Feb 2023 – Aug 2023
- B.S. Pohang University of Science and Technology (POSTECH)**, Computer Science Pohang, South Korea
 and Engineering (CSE) Feb 2020 – Feb 2024

Experience

- Korea Advanced Institute of Science and Technology (KAIST)**, Grant Recipient
 Research Encouragement Grant for Graduate Students (Selected)
 - Inference-Time Steering of Biomolecular Diffusion Models using Feynman-Kac based Diffusion Samplers
- Pohang University of Science and Technology (POSTECH)**, Research intern Aug 2024 – Feb 2025
 Boltzmann sampling via Harmonic Path Integral Diffusion
 - Coworkers: Sungsoo Ahn, Michael Chertkov, Hamidreza Behjoo

Skills

Programming: C++, Python

Tools: PyTorch, Pymatgen, ASE, Pymatgen, OpenMM, Fairchem

Fundamentals: Generative Models, Equivariant Networks, Reinforcement Learning, Stochastic Differential Equations