Minkyu Kim

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minkyu1022 | minkyu1022 | Google Scholar

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

On scalable and efficient training of diffusion samplers 2025
Minkyu Kim, Kiyoung 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***, Kiyoung Seong, Sungsoo Ahn
arxiv.org/abs/2505.19646 (NeurIPS 2025)

Education

Ph.D. **Korea Advanced Institute of Science and Technology (KAIST)**, Kim Jaechul Gradudate School of Artificial Intelligence — Seoul, South Korea, 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, Feb 2023 – Aug 2023
Exchange Student

B.S. **Pohang University of Science and Technology (POSTECH)**, Computer Science and Engineering (CSE) — Pohang, South Korea, Feb 2020 – Feb 2024

Experience

Korea Advanced Institute of Science and Technology (KAIST), Project leader — Aug 2025 – present
Catalyst Generation Conditioned on Adsorbates via Diffusion (Ongoing)
- Designing a one-shot generative model to jointly predict slab stoichiometry (element counts/ratios) and structure directly from elemental composition.

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 Differntial Equations