

Minkyu Kim

📍 Seoul, South Korea ✉️ minkyu-kim@kaist.ac.kr 📞 010-6342-9959 🔗 minkyu1022.github.io/mkkim
linkedin minkyu1022 ORCID 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 ↗](https://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 ↗](https://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. Institut National des Sciences Appliquées (INSA) Lyon**, Bioinfomatics Vienna, Austria
Exchange Student Feb 2023 – Aug 2023
- 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 Scaling of Biomolecular Diffusion Models using Feynman-Kac based Search-Guided 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