Seonghyun Park

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Summary

I'm a second-year Ph.D. student at Graduate School of AI at KAIST, advised by Sungsoo Ahn. Currently, my research focuses on **AI for Science (AI4Science)**, specifically integrating machine learning with biomolecular modeling and molecular dynamics (MD). Recently, I led a project on machine learning–based Collective Variables (CVs) for enhanced sampling of proteins, by repurposing foundation models. Before, my Master's research focused on addressing the over-squashing phenomenon in Graph Neural Networks (GNNs) to capture long-range interactions in molecule graphs.

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
- Interest: Bio-molecules, Molecular dynamics (MD)

M.S. **Pohang University of Science and Technology (POSTECH)**, Graduate School of Computer Science and Engineering (CSE) — Pohang, South Korea, Feb 2023 – Feb 2025
- Machine Learning Lab @ Sungsoo Ahn
- Interest: Graph Neural Networks (GNNs), Over-squashing

E.S. **Institut National des Sciences Appliquées (INSA) Lyon**, Bioinfomatics Exchange Student — Lyon, France, Jan 2022 – June 2022

B.S. **Pohang University of Science and Technology (POSTECH)**, Computer Science and Engineering (CSE) — Pohang, South Korea, Feb 2019 – Feb 2023

Experience

Bagelcode, Buisness Analyst (BA) intern — Seoul, South Korea, June 2021 – Aug 2021
Game economy management and KPI analysis automation

Seller Hub, Product Manager (PM) intern — Seoul, South Korea, July 2020 – Aug 2020
Organization-wide task prioritization and landing funnel renewal

Publication

INDIBATOR: Diverse and Fact-Grounded Individuality for Multi-Agent Debate in Molecular Discovery — 2026
Yunhui Jang, ***Seonghyun Park***, Jaehyung Kim, Sungsoo Ahn
10.48550/arXiv.2602.01815 (Preprint)

Riemannian MeanFlow — 2026
Dongyeop Woo, Marta Skreta, ***Seonghyun Park***, Kirill Neklyudov, Sungsoo Ahn
10.48550/arXiv.2602.07744 (Preprint)

Boltz is a Strong Baseline for Atom-level Representation Learning — 2026
Hyosoon Jang, Hyunjin Seo, Yunhui Jang, ***Seonghyun Park***, Sungsoo Ahn
10.48550/arXiv.2602.13249 (Preprint)

Learning Collective Variables from BioEmu with Time-lagged Generation — Apr 2026
Seonghyun Park, Kiyoung Seong, Soojung Yang, Rafael Gomez-Bombarelli, Sungsoo Ahn
10.48550/arXiv.2507.07390 (ICLR 2026)

Transition Path Sampling with Improved Off-Policy Training of Diffusion Path Samplers Apr 2025

Kiyoung Seong, ***Seonghyun Park***, Seonghwan Kim, Woo Youn Kim, Sungsoo Ahn

10.48550/arXiv.2405.19961 (ICLR 2025)

Non-backtracking Graph Neural Networks Sep 2024

Seonghyun Park*, Narae Ryu*, Gahee Kim, Dongyeop Woo, Se-Young Yun**, Sungsoo Ahn**

10.48550/arXiv.2310.07430 (TMLR 2024, NeurIPS 2023 Workshop GLFrontiers Oral)

Diffusion Probabilistic Models for Structured Node Classification Nov 2023

Hyosoon Jang, ***Seonghyun Park***, Sangwoo Mo, Sungsoo Ahn

10.48550/arXiv.2302.10506 (NeurIPS 2023)