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Summary

I'm a second-year Ph.D. candidate at Graduate School of AI at KAIST, advised by [Sungsoo Ahn](#). My Master's research focused on addressing the over-squashing phenomenon in Graph Neural Networks (GNNs) to capture long-range interactions in molecule graphs. 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.

Publication

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| Learning Collective Variables from BioEmu with Time-lagged Generation | 2026 |
| <i>Seonghyun Park</i> , Kiyong Seong, Soojung Yang, Rafael Gomez-Bombarelli, Sungsoo Ahn
ICLR 2026 | |
| Transition Path Sampling with Improved Off-Policy Training of Diffusion Path Samplers | 2025 |
| Kiyong Seong, <i>Seonghyun Park</i> , Seonghwan Kim, Woo Youn Kim, Sungsoo Ahn
iclr.cc/virtual/2025/poster/29361 (ICLR 2025) | |
| Non-backtracking Graph Neural Networks | 2024 |
| <i>Seonghyun Park*</i> , Narae Ryu*, Gahee Kim, Dongyeop Woo, Se-Young Yun**, Sungsoo Ahn**
arxiv.org/abs/2310.07430 (TMLR 2024, NeurIPS 2023 GLFrontiers Workshop (Oral)) | |
| Diffusion Probabilistic Models for Structured Node Classification | 2023 |
| Hyosoon Jang, <i>Seonghyun Park</i> , Sangwoo Mo, Sungsoo Ahn
neurips.cc/virtual/2023/poster/72405 (NeurIPS 2023) | |

Education

- | | |
|---|--|
| Ph.D. Korea Advanced Institute of Science and Technology (KAIST) , Kim Jaechul
Graduate School of Artificial Intelligence | Seoul, South Korea
Feb 2025 – present |
| <ul style="list-style-type: none"> 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 |
| <ul style="list-style-type: none"> Machine Learning Lab @ Sungsoo Ahn Interest: Graph Neural Networks (GNNs), Over-squashing | |
| E.S. Institut National des Sciences Appliquées (INSA) Lyon , Bioinformatics
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

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|--|--|
| Bagelcode , Buisness Analyst (BA) intern
KPI routines automation and game economy management | Seoul, South Korea
June 2021 – Aug 2021 |
| Seller Hub , Product Manager (PM) intern
Task priority management and landing page renewal | Seoul, South Korea
July 2020 – Aug 2020 |