

# Seonghyun Park

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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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| <b>Learning Collective Variables from BioEmu with Time-lagged Generation</b>   | 2026 |
| <i>Seonghyun Park</i> , Kiyong Seong, Soojung Yang, Rafael Gomez-Bombarelli, Sungsoo Ahn<br><a href="https://openreview.net/forum?id=1PYj4fMeLe">openreview.net/forum?id=1PYj4fMeLe</a> (ICLR 2026)                          |      |
| <b>Transition Path Sampling with Improved Off-Policy Training of Diffusion Path Samplers</b>   | 2025 |
| Kiyong Seong, <i>Seonghyun Park</i> , Seonghwan Kim, Woo Youn Kim, Sungsoo Ahn<br><a href="https://iclr.cc/virtual/2025/poster/29361">iclr.cc/virtual/2025/poster/29361</a> (ICLR 2025)                                      |      |
| <b>Non-backtracking Graph Neural Networks</b>  | 2024 |
| <i>Seonghyun Park*</i> , Narae Ryu*, Gahee Kim, Dongyeop Woo, Se-Young Yun**, Sungsoo Ahn**<br><a href="https://arxiv.org/abs/2310.07430">arxiv.org/abs/2310.07430</a> (TMLR 2024, NeurIPS 2023 GLFrontiers Workshop (Oral)) |      |
| <b>Diffusion Probabilistic Models for Structured Node Classification</b>   | 2023 |
| Hyosoon Jang, <i>Seonghyun Park</i> , Sangwoo Mo, Sungsoo Ahn<br><a href="https://neurips.cc/virtual/2023/poster/72405">neurips.cc/virtual/2023/poster/72405</a> (NeurIPS 2023)  |      |

## Education

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|---|--|
| <b>Ph.D. Korea Advanced Institute of Science and Technology (KAIST)</b> , Kim Jaechul<br>Graduate School of Artificial Intelligence   | Seoul, South Korea<br>Feb 2025 – present   |
| <ul style="list-style-type: none"> <li>• <a href="#">Structured and Probabilistic Machine Learning Lab</a> @ Sungsoo Ahn</li> <li>• Interest: Bio-molecules, Molecular dynamics (MD)</li> </ul> |  |
| <b>M.S. Pohang University of Science and Technology (POSTECH)</b> , Graduate School of<br>Computer Science and Engineering (CSE)  | Pohang, South Korea<br>Feb 2023 – Feb 2025 |
| <ul style="list-style-type: none"> <li>• <a href="#">Machine Learning</a> Lab @ Sungsoo Ahn</li> <li>• Interest: Graph Neural Networks (GNNs), Over-squashing</li> </ul>                        |  |
| <b>E.S. Institut National des Sciences Appliquées (INSA) Lyon</b> , Bioinformatics<br>Exchange Student  | Lyon, France<br>Jan 2022 – June 2022       |
| <b>B.S. Pohang University of Science and Technology (POSTECH)</b> , Computer Science<br>and Engineering (CSE)   | Pohang, South Korea<br>Feb 2019 – Feb 2023 |

## Experience

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