Kiyoung Seong

email | linkedin | github | homepage

Education

KAIST — Seoul, South Korea
Ph.D. Student, Structured and Probabilistic Machine Learning Lab (Advisor: Sungsoo Ahn) — *Mar. 2025 – Present*

Korea University — Seoul, South Korea
B.S. in Mathematics Education, Advanced Mathematics Track — *Mar. 2017 – Feb. 2023*

Experience

POSTECH — Pohang, South Korea
Researcher — *June 2023 – Feb. 2025*

LG AI Research — Seoul, South Korea
Research Intern in Materials Intelligence Lab — *Sep. 2025 – Feb. 2026*

Research Projects

Multimodal Crystal Flow: Any-to-Any Modality Generation for Unified Crystal Modeling | *ICML* 2026
- **Goal**: Unify de novo generation, structure prediction, and atom type generation in one model.
- **Role**: (1) Led the project as first author, and (2) designed a multimodal flow with symmetry-aware ordering.
- **Result**: Matched task-specific baselines on MP-20 and MPTS-52.
- Used: PyTorch

Transition Path Sampling with Improved Off-Policy Training of Diffusion Path Samplers | *ICLR* 2025
- **Goal**: Sampling transition between metastable states to understand the mechanism and calculate observables.
- **Role**: (1) Led the project as first author, and (2) developed an off-policy transition path sampling algorithm.
- **Result**: 84% improvement in sampling paths of the BBA protein over prior baselines.
- Used: PyTorch, OpenMM

On Scalable and Efficient Training of Diffusion Samplers | *NeurIPS* 2025
- **Goal**: Sampling a state in a data-free setting where only energy evaluation is available.
- **Role**: (1) Led the project as co-first author, and (2) developed equivariant generative model to sample from MLIP.
- **Result**: Outperformed prior baselines with 0.1% of the energy evaluations on Lennard-Jones; sampled di-, tri-, tetra-peptide conformations with MLIP.
- Used: PyTorch, TorchANI, ASE

Learning Collective Variables from BioEmu with Time-Lagged Generation | *ICLR* 2026
- **Goal**: Learn slow degrees of freedom of molecules from a conformation ensemble generative model (BioEmu).
- **Role**: Designed and implemented a transition path sampling experiment to evaluate collective variables (CVs).
- **Result**: 75% improvement in sampling paths of the BBA protein over prior CV baselines.
- Used: PyTorch, OpenMM

Technical Skills

Machine Learning: Generative Models, Equivariant Networks, Reinforcement Learning, AI for Molecular Dynamics
Programming: Python
Libraries: PyTorch, OpenMM, FAIRChem, TorchANI

Invited Talks

KAIST 2025 AI Technology Symposium — Coex, Seoul, South Korea
Speaker — *May 2025*