

Dongki Kim

[Homepage](#) | [GitHub](#) | [Google Scholar](#) | [Twitter](#)

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SUMMARY

I am a second-year PhD student advised by Sung Ju Hwang. I am interested in solving scientific problems with the purpose of enhancing our understanding of biomolecules and their complex system and the generation of biomolecular structures. I have been working on representation learning, diffusion models, and large language models for biomolecular structures.

EDUCATION

KAIST

Ph.D. in Artificial Intelligence

M.S. in Artificial Intelligence

- Advisor: [Prof. Sung Ju Hwang](#)

Deajeon, South Korea

Sep. 2023 – Present

Sep. 2021 – Aug. 2023

Seoul National University (SNU)

B.S. in Compute Science and Engineering

B.S. in Applied Life Chemistry

Seoul, South Korea

Mar. 2014 – Feb. 2021

Mar. 2014 – Feb. 2021

PUBLICATION

Mol-LLaMA: Towards General Understanding of Molecules in Large Molecular Language Model

[Dongki Kim](#), Wonbin Lee, Sung Ju Hwang

Preprint, 2025

Graph Generation with Diffusion Mixture

Jaehyeong Jo*, [Dongki Kim](#)*, Sung Ju Hwang

International Conference on Machine Learning (ICML), 2024

Machine Learning for Drug Discovery Workshop at ICLR (MLDD @ ICLR), 2023 (Spotlight)

Protein Representation Learning by Capturing Protein Sequence-Structure-Function Relationship

Eunji Ko*, Seul Lee*, Minseon Kim*, [Dongki Kim](#), Sung Ju Hwang

Machine Learning for Genomics Explorations Workshop at ICLR (MLGenX @ ICLR), 2024 (Spotlight)

Antibody-SGM: Antigen-Specific Joint Design of Antibody Sequence and Structure using Diffusion Models

Xuezhi Xie, Jin Sub Lee, [Dongki Kim](#), Jaehyeong Jo, Jisun Kim, Philip M. Kim

Computational Biology Workshop at ICML (CompBio @ ICML), 2023

Graph Self-supervised Learning with Accurate Discrepancy Learning

[Dongki Kim](#)*, Jinheon Baek*, Sung Ju Hwang

Conference on Neural Information Processing Systems (NeurIPS), 2022

Edge Representation Learning with Hypergraphs

Jaehyeong Jo*, Jinheon Baek*, Seul Lee*, [Dongki Kim](#), Minki Kang, Sung Ju Hwang

Conference on Neural Information Processing Systems (NeurIPS), 2021

* denotes equal contribution

RESEACH EXPERIENCE

MLAI Lab, KAIST

Mar. 2021 – Present

Research Assistant (Advisor: Prof. Sung Ju Hwang)

- Conducting research on graph-structured data for representation learning and generation with the application to the molecular and general graphs.

Kim Lab, University of Toronto

Feb. 2023 – Feb. 2023

Visiting Student (Host: Prof. Philip M. Kim)

- Conducting research on protein generation using diffusion models.

TALK

Generation of Graph-Structured Data with Diffusion Models

at University of Toronto

Feb. 2023

Graph Self-supervised Learning with Accurate Discrepancy Learning

at KAIST

Nov. 2022

ACADEMIC SERVICE

Conference Reviewer

- International Conference on Machine Learning (**ICML**), 2025
- Transactions on Machine Learning Research (**PMLR**), 2025
- International Conference on Learning Representations (**ICLR**), 2025
- Generative and Experimental Perspectives for Biomolecular Design Workshop at ICLR (**GEM @ ICLR**), 2025
- Conference on Neural Information Processing Systems (**NeurIPS**), 2024
- International Conference on Machine Learning (**ICML**), 2024
- International Conference on Learning Representations (**ICLR**), 2024
- Generative and Experimental Perspectives for Biomolecular Design Workshop at ICLR (**GEM @ ICLR**), 2024
- Conference on Neural Information Processing Systems (**NeurIPS**), 2023
- International Conference on Machine Learning (**ICML**), 2023
- Conference on Neural Information Processing Systems (**NeurIPS**), 2022
- International Conference on Machine Learning (**ICML**), 2022

REFERENCE

- [Prof. Sung Ju Hwang](#), Endowed Chair Professor, KAIST
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