# Dongki Kim

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## SUMMARY

I am a third-year PhD student advised by Sung Ju Hwang. I have been working on the intersections of AI and life science, bridging their gap by modeling biomolecules and their complex system via representation learning, generative models, and LLMs.

## EDUCATION

**KAIST** — **Deajeon, South Korea**
Ph.D. in Artificial Intelligence — *Sep. 2023 – Present*
M.S. in Artificial Intelligence — *Sep. 2021 – Aug. 2023*
- Advisor: Prof. Sung Ju Hwang

**Seoul National University (SNU)** — **Seoul, South Korea**
B.S. in Compute Science and Engineering — *Mar. 2014 – Feb. 2021*
B.S. in Applied Biology and Chemistry — *Mar. 2014 – Feb. 2021*

## PUBLICATION

**Multimodal Prompt Optimization: Why Not Leverage Multiple Modalities for MLLMs**
Yumin Choi*, Dongki Kim*, Jinheon Baek, Sung Ju Hwang
International Conference on Learning Representations (**ICLR**), 2026

**Mol-LLaMA: Towards General Understanding of Molecules in Large Molecular Language Model**
Dongki Kim, Wonbin Lee, Sung Ju Hwang
Conference on Neural Information Processing Systems (**NeurIPS**), 2025
AI for Science Workshop at NeurIPS (**AI4Science @ NeurIPS**), 2025

**Graph Generation with Diffusion Mixture**
Jaeheyong Jo*, Dongki Kim*, Sung Ju Hwang
International Conference on Machine Learning (**ICML**), 2024
ML 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
ML 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

## PREPRINT

**Rethinking Reward Models for Multi-Domain Test-Time Scaling**
Dong Bok Lee*, Seanie Lee*, Sangwoo Park, Minki Kang, Jinheon Baek, Dongki Kim, Dominik Wagner, Jiongdao Jin, Heejun Lee, Tobias Bocklet, Jinyu Wang, Jingjing Fu, Sung Ju Hwang, Jiang Bian, Lei Song
Preprint, 2025

## RESEACRH 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

**Towards General Understanding of Molecules in Large Molecular Language Model**
at KAIST *May. 2025*

**Explainable PK/Tox Prediction: Molecular-Protein-Language Tri-modality Foundation Model**
at Korea Machine Learning Ledger Orchestration for Drug Discovery *March. 2025*

**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
- Conference on Neural Information Processing Systems (**NeurIPS**), *2025*
- 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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