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

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

Multimodal Prompt Optimization: Why Not Leverage Multiple Modalities for MLLMs
Yumin Choi*, Dongki Kim*, Jinheon Baek, Sung Ju Hwang
Preprint, 2025

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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