Dongki Kim

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RESEARCH INTERESTS

My research primarily focuses on deep learning models to enhance our understanding of molecules and aid in molecular design. I have been working on diffusion models and representation learning for graph structures, particularly with applications to biomolecules.

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 Life Chemistry — *Mar. 2014 – Feb. 2021*

PUBLICATION

Graph Generation with Diffusion Mixture
Jaeheyong 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

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

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 Learning Representations (**ICLR**), *2025*
- Conference on Neural Information Processing Systems (**NeurIPS**), *2024*
- International Conference on Machine Learning (**ICML**), *2024*
- International Conference on Learning Representations (**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
  E-mail: sjhwang82@kaist.ac.kr