

Seul Lee

CONTACT INFORMATION

KAIST, Seoul, South Korea
E-mail: seul.lee@kaist.ac.kr
Homepage: seullee05.github.io

RESEARCH INTERESTS

My research interest is mainly in developing an automated discovery framework for organic molecules, natural products, or proteins. I especially focus on molecule generation that can bridge the gap between real-world drug discovery and automatic drug discovery. I am currently interested in the following topics:

- AI for science
- Drug discovery
- Generative models
- Graph representation learning

EDUCATION

KAIST, Seoul, South Korea

Ph.D. student, Graduate School of AI **Sep. 2022 - present**

- Advisor: Prof. Sung Ju Hwang
- Area of study: Machine learning
- Expected graduation date: Aug. 2026

M.S., Graduate School of AI **Mar. 2021 - Aug. 2022**

- Advisor: Prof. Sung Ju Hwang
- Area of study: Machine learning
- GPA: 4.20/4.3

B.S., Aerospace Engineering **Mar. 2015 - Aug. 2019**

- Double Major in Biological Sciences
- GPA: 4.18/4.3

RESEARCH EXPERIENCE

NVIDIA Research **Feb. 2024 - Aug. 2024**

- Location: Santa Clara, CA, US (remote)
- Position: Research intern
- Research topic: Generative AI for science

Kimlab & The Matter Lab, UofT **Jun. 2023 - Jun. 2023**

- Location: Toronto, Canada
- Position: Visiting researcher
- Host: Prof. Philip M. Kim & Prof. Alán Aspuru-Guzik

AITRICS

Jan. 2021 - Feb. 2021

- Location: Seoul, South Korea
- Position: Research intern
- Research topic: Docking-optimized molecule generation using RL

Opto-Electro-Robotics Lab, KAIST

Mar. 2019 - Aug. 2019

- Location: Daejeon, South Korea
- Position: Undergraduate researcher
- Advisor: Prof. Jung-ryul Lee
- Research topic: Laser pulse-echo inspection with robot arms

INVITED TALKS

- Exploring Chemical Space with Score-based OOD Generation, **Nov. 2023**
Hyundai 2023 CTO AI Conference
- Exploring Chemical Space with Score-based OOD Generation, **Jun. 2023**
University of Toronto
- Score-based Generative Modeling of Graphs via the SDEs, **Oct. 2022**
LoGaG: Learning on Graphs and Geometry Reading Group
- Learning with Graph-structured Data, POSTECH **Jul. 2022**
- Score-based Graph Generation for Material Design, **Jun. 2022**
Samsung Advanced Institute of Technology (SAIT)

CONFERENCE PUBLICATIONS

- [c5] **A Simple and Scalable Representation for Graph Generation**
Yunhui Jang, **Seul Lee**, and Sungsoo Ahn,
International Conference on Learning Representations (ICLR), 2024.
- [c4] **Exploring Chemical Space with Score-based Out-of-distribution Generation**
Seul Lee, Jaehyeong Jo, and Sung Ju Hwang,
International Conference on Machine Learning (ICML), 2023.
- [c3] **Score-based Generative Modeling of Graphs via the System of Stochastic Differential Equations**
Jaehyeong Jo*, **Seul Lee***, and Sung Ju Hwang (*: equal contribution),
International Conference on Machine Learning (ICML), 2022.
- [c2] **Edge Representation Learning with Hypergraphs**
Jaehyeong Jo*, Jinheon Baek*, **Seul Lee***, Dongki Kim, Minki Kang, and Sung Ju Hwang (*: equal contribution),
Conference on Neural Information Processing Systems (NeurIPS), 2021.
- [c1] **Hit and Lead Discovery with Explorative RL and Fragment-based Molecule Generation**
Soojung Yang, Doyeong Hwang, **Seul Lee**, Seongok Ryu, and Sung Ju Hwang,
Conference on Neural Information Processing Systems (NeurIPS), 2021.

JOURNAL
PUBLICATIONS

- [j1] **Robotic Scanning Technology for Laser Pulse-Echo Inspection**
Seul Lee, Jong-min Hyun, Hasan Ahmed, and Jung-ryul Lee,
Electronics Letters, 2020.

WORKSHOP
PUBLICATIONS

- [w4] **Protein Representation Learning by Capturing Protein Sequence-Structure-Function Relationship**
Eunji Ko*, Seul Lee*, Minseon Kim*, Dongki Kim, and Sung Ju Hwang (*: equal contribution),
International Conference on Learning Representation Machine Learning for Genomics Explorations (**ICLR MLGenX) Workshop (Spotlight), 2024.**
- [w3] **Drug Discovery with Dynamic Goal-aware Fragments**
Seul Lee, Seanie Lee, Kenji Kawaguchi, and Sung Ju Hwang,
International Conference on Learning Representation Machine Learning for Genomics Explorations (**ICLR MLGenX) Workshop (Spotlight), 2024.**
- [w2] **A Simple and Scalable Representation for Graph Generation**
Yunhui Jang, Seul Lee, and Sungsoo Ahn,
Conference on Neural Information Processing Systems New Frontiers in Graph Learning (**NeurIPS GLFrontiers) Workshop, 2023.**
- [w1] **Exploring Chemical Space with Score-based Out-of-distribution Generation**
Seul Lee, Jaehyeong Jo, and Sung Ju Hwang,
International Conference on Learning Representations Machine Learning for Drug Discovery (**ICLR MLDD) Workshop (Oral), 2023.**

PREPRINTS

- [p3] **Protein Representation Learning by Capturing Protein Sequence-Structure-Function Relationship**
Eunji Ko*, Seul Lee*, Minseon Kim*, Dongki Kim, and Sung Ju Hwang (*: equal contribution),
Under Review, 2024.
- [p2] **Drug Discovery with Dynamic Goal-aware Fragments**
Seul Lee, Seanie Lee, Kenji Kawaguchi, and Sung Ju Hwang,
Under Review, 2024.
- [p1] **READRetro: Natural Product Biosynthesis Planning with Retrieval-Augmented Dual-View Retrosynthesis**
Seul Lee*, Taein Kim*, Min-Soo Choi, Yejin Kwak, Jeongbin Park, Sung Ju Hwang, and Sang-Gyu Kim (*: equal contribution),
Under Review, 2024.

REVIEWER SERVICES	<ul style="list-style-type: none"> • 2024 International Conference on Learning Representations (ICLR) • 2022, 2023, 2024 International Conference on Machine Learning (ICML) • 2021, 2023 Conference on Neural Information Processing Systems (NeurIPS) • 2023 Learning on Graphs Conference (LoG) • 2023 NeurIPS AI4Science Workshop • 2023 NeurIPS Generative AI & Biology Workshop • 2023 ICLR ML4Materials Workshop
HONORS AND AWARDS	<ul style="list-style-type: none"> • Boeing Undergraduate Scholarship Feb. 2018 - Aug. 2019 • KAIST Presidential Fellowship (KPF) Mar. 2017 - Aug. 2019 • National Science and Engineering Scholarship Mar. 2015 - Feb. 2019
REFERENCES	<ul style="list-style-type: none"> • Prof. Sung Ju Hwang, KAIST <i>E-mail:</i> sjhwang82@kaist.ac.kr