

Seul Lee

CONTACT INFORMATION KAIST, Seoul, South Korea
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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

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
- GPA: 4.3/4.3

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

- Advisor: Prof. Sung Ju Hwang
- Area of study: Machine learning
- GPA: 4.2/4.3

B.S., Biological Sciences Mar. 2015 - Aug. 2019

- Double Major in Aerospace Engineering
- GPA: 4.18/4.3

RESEARCH EXPERIENCE **NVIDIA** Feb. 2024 - Sep. 2025

- [Fundamental Generative AI Research \(GenAIR\) Team](#)
- Location: Santa Clara, CA, US
- 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

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**

- [c7] **Molecule Generation with Fragment Retrieval Augmentation**
Seul Lee, Karsten Kreis, Srimukh Prasad Veccham, Meng Liu, Danny Reidenbach, Saeed Paliwal, Arash Vahdat[†], and Weili Nie[†] ([†]: equal advising),
Conference on Neural Information Processing Systems (**NeurIPS**), **2024**.
- [c6] **Drug Discovery with Dynamic Goal-aware Fragments**
Seul Lee, Seanie Lee, Kenji Kawaguchi, and Sung Ju Hwang,
International Conference on Machine Learning (**ICML**), **2024**.
- [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	[j2] READRetro: Natural Product Biosynthesis Planning with Retrieval-Augmented Dual-View Retrosynthesis Taein Kim*, Seul Lee* , Min-Soo Choi, Yejin Kwak, Jeongbin Park, Sung Ju Hwang, and Sang-Gyu Kim (*: equal contribution), New Phytologist , 2024.
	[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	[p1] GenMol: A Drug Discovery Generalist with Discrete Diffusion Seul Lee , Karsten Kreis, Srirukh Prasad Veccham, Meng Liu, Danny Reidenbach, Yuxing Peng, Saeed Paliwal, Weili Nie [†] , and Arash Vahdat [†] (†: equal advising), 2025.
REVIEWER SERVICES	<ul style="list-style-type: none"> • 2024, 2025 International Conference on Learning Representations (ICLR) • 2022, 2023, 2024 International Conference on Machine Learning (ICML) • 2021, 2023, 2024 Conference on Neural Information Processing Systems (NeurIPS) • 2023, 2024 Learning on Graphs Conference (LoG) • 2023 NeurIPS AI4Science Workshop • 2023 NeurIPS Generative AI & Biology Workshop • 2023 ICLR ML4Materials Workshop

HONORS AND AWARDS	• NVIDIA Graduate Fellowship	2025 - 2026
	• Boeing Undergraduate Scholarship	2018 - 2019
	• KAIST Presidential Fellowship (KPF)	2017 - 2019
	• National Science and Engineering Scholarship	2015 - 2019

REFERENCES • [Prof. Sung Ju Hwang](#), KAIST
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