

Seul Lee

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RESEARCH My research interest is mainly in developing an automated discovery framework
INTERESTS 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 **NVIDIA** **Feb. 2024 - Jun. 2025**
EXPERIENCE

- 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

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

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

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 Ge-
nomics 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 Ge-
nomics 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**.

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|-------------------|--|---|
| 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 | <ul style="list-style-type: none"> • Boeing Undergraduate Scholarship • KAIST Presidential Fellowship (KPF) • National Science and Engineering Scholarship | <p>Feb. 2018 - Aug. 2019</p> <p>Mar. 2017 - Aug. 2019</p> <p>Mar. 2015 - Feb. 2019</p> |
| REFERENCES | <ul style="list-style-type: none"> • Prof. Sung Ju Hwang, KAIST <i>E-mail:</i> sjhwang82@kaist.ac.kr | |