Seul Lee

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

<small>RESEARCH INTERESTS</small>

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

<small>EDUCATION</small>

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

<small>RESEARCH EXPERIENCE</small>

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

[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**
Seul Lee*, Taein Kim*, 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] **Molecule Generation with Fragment Retrieval Augmentation**
Seul Lee, Karsten Kreis, Srimukh Prasad Veccham, Meng Liu, Danny Reidenbach, Saee Paliwal, Arash Vahdat[†], and Weili Nie[†] (†: equal advising),
Under Review, 2024.

REVIEWER SERVICES

- 2024 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	• 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

- Prof. Sung Ju Hwang, KAIST
  E-mail: sjhwang82@kaist.ac.kr