Seul Lee

CONTACT INFORMATION

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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 - Jun. 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

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, 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, Saee 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**.

Reviewer Services

- 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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