# Seul Lee

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| CONTACT INFORMATION | KAIST, Seoul, South Korea<br>*E-mail:* seul.lee@kaist.ac.kr<br>*Homepage:* seullee05.github.io<br>*Google Scholar:* Seul Lee |

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 (but not limited to) the following topics:

- AI for science
- Generative models
- Drug discovery

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: 4.27/4.3

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

- Advisor: Prof. Sung Ju Hwang
- Area of study: Machine learning
- GPA: 4.26/4.3

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 small molecules

**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

- Towards a Generalist Model for Molecule Generation,　　　**Apr. 2025**
  San Francisco Bay Area COMP Together
- 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

[c8] **GenMol: A Drug Discovery Generalist with Discrete Diffusion**

**Seul Lee**, Karsten Kreis, Srimukh Prasad Veccham, Meng Liu, Danny Reidenbach, Yuxing Peng, Saee Paliwal, Weili Nie[†], and Arash Vahdat[†] (†: equal advising), International Conference on Machine Learning **(ICML), 2025**.

[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**.

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| ACADEMIC SERVICES | • Co-organizer of 2025 ICML Generative AI and Biology (GenBio) Workshop |
| | • Reviewer of |
| | 2024, 2025 International Conference on Learning Representations (ICLR) |
| | 2022, 2023, 2024, 2025 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 |

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| 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** |

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