

## Seul Lee

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CONTACT INFORMATION KAIST, Seoul, South Korea  
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*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: 4.3/4.3

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 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, Srividya Prasad Veccham, Meng Liu, Danny Reidenbach, Yuxing Peng, Saeed Paliwal, Weili Nie<sup>†</sup>, and Arash Vahdat<sup>†</sup> (<sup>†</sup>: equal advising), International Conference on Machine Learning (ICML), **2025**.
- [c7] **Molecule Generation with Fragment Retrieval Augmentation**  
**Seul Lee**, Karsten Kreis, Srividya Prasad Veccham, Meng Liu, Danny Reidenbach, Saeed Paliwal, Arash Vahdat<sup>†</sup>, and Weili Nie<sup>†</sup> (<sup>†</sup>: 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**, Jaehyeon 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**  
Jaehyeon 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**.

ACADEMIC SERVICES	<ul style="list-style-type: none"> <li>• Co-organizer of <a href="#">2025 ICML Generative AI and Biology (GenBio) Workshop</a></li> <li>• Reviewer of <ul style="list-style-type: none"> <li>2024, 2025 International Conference on Learning Representations (ICLR)</li> <li>2022, 2023, 2024, 2025 International Conference on Machine Learning (ICML)</li> <li>2021, 2023, 2024 Conference on Neural Information Processing Systems (NeurIPS)</li> <li>2023, 2024 Learning on Graphs Conference (LoG)</li> <li>2023 NeurIPS AI4Science Workshop</li> <li>2023 NeurIPS Generative AI &amp; Biology Workshop</li> <li>2023 ICLR ML4Materials Workshop</li> </ul> </li> </ul>
HONORS AND AWARDS	<ul style="list-style-type: none"> <li>• <a href="#">NVIDIA Graduate Fellowship</a> <b>2025 - 2026</b></li> <li>• Boeing Undergraduate Scholarship <b>2018 - 2019</b></li> <li>• KAIST Presidential Fellowship (KPF) <b>2017 - 2019</b></li> <li>• National Science and Engineering Scholarship <b>2015 - 2019</b></li> </ul>
REFERENCES	<ul style="list-style-type: none"> <li>• <a href="#">Prof. Sung Ju Hwang</a>, KAIST <i>E-mail:</i> <a href="mailto:sjhwang82@kaist.ac.kr">sjhwang82@kaist.ac.kr</a></li> </ul>