

## 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**

- 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**

- [c7] **Molecule Generation with Fragment Retrieval Augmentation**  
**Seul Lee**, Karsten Kreis, Srimukh 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**, 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] <b>READRetro: Natural Product Biosynthesis Planning with Retrieval-Augmented Dual-View Retrosynthesis</b> Taein Kim*, <b>Seul Lee*</b> , Min-Soo Choi, Yejin Kwak, Jeongbin Park, Sung Ju Hwang, and Sang-Gyu Kim (*: equal contribution), <b>New Phytologist</b> , 2024.
	[j1] <b>Robotic Scanning Technology for Laser Pulse-Echo Inspection</b> <b>Seul Lee</b> , Jong-min Hyun, Hasan Ahmed, and Jung-ryul Lee, <b>Electronics Letters</b> , 2020.
WORKSHOP PUBLICATIONS	[w4] <b>Protein Representation Learning by Capturing Protein Sequence-Structure-Function Relationship</b> Eunji Ko*, <b>Seul Lee*</b> , Minseon Kim*, Dongki Kim, and Sung Ju Hwang (*: equal contribution), International Conference on Learning Representation Machine Learning for Genomics Explorations ( <b>ICLR MLGenX</b> ) <b>Workshop (Spotlight)</b> , 2024.
	[w3] <b>Drug Discovery with Dynamic Goal-aware Fragments</b> <b>Seul Lee</b> , Seanie Lee, Kenji Kawaguchi, and Sung Ju Hwang, International Conference on Learning Representation Machine Learning for Genomics Explorations ( <b>ICLR MLGenX</b> ) <b>Workshop (Spotlight)</b> , 2024.
	[w2] <b>A Simple and Scalable Representation for Graph Generation</b> Yunhui Jang, <b>Seul Lee</b> , and Sungsoo Ahn, Conference on Neural Information Processing Systems New Frontiers in Graph Learning ( <b>NeurIPS GLFrontiers</b> ) <b>Workshop</b> , 2023.
	[w1] <b>Exploring Chemical Space with Score-based Out-of-distribution Generation</b> <b>Seul Lee</b> , Jaehyeong Jo, and Sung Ju Hwang, International Conference on Learning Representations Machine Learning for Drug Discovery ( <b>ICLR MLDD</b> ) <b>Workshop (Oral)</b> , 2023.
PREPRINTS	[p1] <b>GenMol: A Drug Discovery Generalist with Discrete Diffusion</b> <b>Seul Lee</b> , Karsten Kreis, Srimukh Prasad Veccham, Meng Liu, Danny Reidenbach, Yuxing Peng, Saeed Paliwal, Weili Nie <sup>†</sup> , and Arash Vahdat <sup>†</sup> ( <sup>†</sup> : equal advising), 2025.
ACADEMIC SERVICES	<ul style="list-style-type: none"> <li>• Co-organizer of <b>2025 ICML Generative AI and Biology (GenBio) Workshop</b></li> <li>• 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 &amp; Biology Workshop 2023 ICLR ML4Materials Workshop</li> </ul>

HONORS AND AWARDS	• <a href="#">NVIDIA Graduate Fellowship</a>	<b>2025 - 2026</b>
	• Boeing Undergraduate Scholarship	<b>2018 - 2019</b>
	• KAIST Presidential Fellowship (KPF)	<b>2017 - 2019</b>
	• National Science and Engineering Scholarship	<b>2015 - 2019</b>

REFERENCES • [Prof. Sung Ju Hwang](#), KAIST  
*E-mail:* [sjhwang82@kaist.ac.kr](mailto:sjhwang82@kaist.ac.kr)