Seul Lee

Contact Information

Research Scientist, NVIDIA Fundamental Generative AI Research (GenAIR) Team
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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 (but not limited to) the following topics:

- AI for science
- Generative models
- Drug discovery

Research Experience

NVIDIA **Aug. 2026 - present**

- Fundamental Generative AI Research (GenAIR) Team
- Location: Santa Clara, CA, US
- Position: Research Scientist
- Research topic: Generative AI for small molecules

NVIDIA **Feb. 2024 - Aug. 2026**

- 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

Education

KAIST, Seoul, South Korea

Ph.D. student, Graduate School of AI — **Sep. 2022 - Aug. 2026**

- 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

B.S., Biological Sciences — **Mar. 2015 - Aug. 2019**

- Double Major in Aerospace Engineering

Invited Talks

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

[c10] **Synthon Contrastive Learning for Synthesizable 3D Molecule Generation**

Nahyun Kim*, **Seul Lee***, and Sung Ju Hwang (*: equal contribution), Conference on Neural Information Processing Systems **(NeurIPS), 2026**.

[c9] **Exploring Synthesizable Chemical Space with Iterative Pathway Refinements**

Seul Lee, Karsten Kreis, Srimukh Prasad Veccham, Meng Liu, Danny Reidenbach, Saee Paliwal, Weili Nie†, and Arash Vahdat† (†: equal advising), International Conference on Learning Representations **(ICLR), 2026 (Oral presentation)**.

[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

[w5] **Synthon Contrastive Learning for Synthesizable 3D Molecule Generation**

Nahyun Kim*, **Seul Lee***, and Sung Ju Hwang (*: equal contribution),
International Conference on Machine Learning Generative and Agentic AI for Biology **(ICML GenBio) Workshop, 2026**.

[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**.

Academic Services

- Co-organizer of 2026 ICML Structured Probabilistic Inference & Generative Modeling (SPIGM) Workshop
- Co-organizer of 2025 ICML Generative AI and Biology (GenBio) Workshop
- Reviewer of
  2021, 2023, 2024, 2025 Conference on Neural Information Processing Systems (NeurIPS)
  2022, 2023, 2024, 2025 International Conference on Machine Learning (ICML)
  2024, 2025 International Conference on Learning Representations (ICLR)
  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**