

Seul Lee

CONTACT INFORMATION

KAIST, Seoul, South Korea
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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
- Graph representation learning

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

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

- Advisor: Prof. Sung Ju Hwang
- Area of study: Machine learning
- GPA: 4.20/4.3

B.S., Aerospace Engineering **Mar. 2015 - Aug. 2019**

- Double Major in Biological Sciences
- GPA: 4.18/4.3

RESEARCH EXPERIENCE

NVIDIA Research **Feb. 2024 - Aug. 2024**

- Location: Santa Clara, CA, US (remote)
- 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

[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	[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	[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.
PREPRINTS	[p3] Protein Representation Learning by Capturing Protein Sequence-Structure-Function Relationship Eunji Ko*, Seul Lee* , Minseon Kim*, Dongki Kim, and Sung Ju Hwang (*: equal contribution), Under Review, 2024. [p2] Drug Discovery with Dynamic Goal-aware Fragments Seul Lee , Seanie Lee, Kenji Kawaguchi, and Sung Ju Hwang, Under Review, 2024. [p1] READRetro: Natural Product Biosynthesis Planning with Retrieval-Augmented Dual-View Retrosynthesis Seul Lee* , Taein Kim*, Min-Soo Choi, Yejin Kwak, Jeongbin Park, Sung Ju Hwang, and Sang-Gyu Kim (*: equal contribution), Under Review, 2024.
REVIEWER SERVICES	<ul style="list-style-type: none"> • 2024 International Conference on Learning Representations (ICLR) • 2022, 2023, 2024 International Conference on Machine Learning (ICML) • 2021, 2023 Conference on Neural Information Processing Systems (NeurIPS) • 2023 Learning on Graphs Conference (LoG) • 2023 NeurIPS AI4Science Workshop • 2023 NeurIPS Generative AI & Biology Workshop • 2023 ICLR ML4Materials Workshop
HONORS AND AWARDS	<ul style="list-style-type: none"> • Boeing Undergraduate Scholarship Feb. 2018 - Aug. 2019 • KAIST Presidential Fellowship (KPF) Mar. 2017 - Aug. 2019 • National Science and Engineering Scholarship Mar. 2015 - Feb. 2019
REFERENCES	<ul style="list-style-type: none"> • Prof. Sung Ju Hwang, KAIST <i>E-mail: sjhwang82@kaist.ac.kr</i>