

## Seul Lee

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### CONTACT INFORMATION

KAIST, Seoul, South Korea  
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### RESEARCH INTERESTS

My research interest is mainly in developing generative models for graphs. 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:

- Drug discovery
- Generative models, especially score-based diffusion 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

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

- Advisor: Prof. Sung Ju Hwang
- Area of study: Machine learning

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

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

### RESEARCH EXPERIENCE

**AITRICS**, Seoul, South Korea

- Research topic: Docking-optimized molecule generation using reinforcement learning

### CONFERENCE PUBLICATIONS

**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**.

**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**.

## 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

**Robotic Scanning Technology for Laser Pulse-Echo Inspection**  
**Seul Lee**, Jong-min Hyun, Hasan Ahmed, and Jung-ryul Lee,  
**Electronics Letters**, **2020**.

### PREPRINTS

**Exploring Chemical Space with Score-based Out-of-distribution Generation**  
**Seul Lee**, Jaehyeong Jo, and Sung Ju Hwang,  
arXiv:2206.07632, 2022.

### HONORS AND AWARDS

- Boeing Undergraduate Scholarship **Feb. 2018 - Aug. 2019**
- KAIST Presidential Fellowship (KPF) **Mar. 2017 - Aug. 2019**
- National Science and Engineering Scholarship **Mar. 2015 - Feb. 2019**

### SKILLS

- Fluent in English
- Fluent in Python and PyTorch

### REFERENCES

- [Prof. Sung Ju Hwang](#), Professor, KAIST  
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