

Seul Lee

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 diffusion models
- Graph representation learning

EDUCATION

KAIST, Daejeon, South Korea

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

- Advisor: Prof. Sung Ju Hwang
- Area of study: Machine learning
- Anticipate proceeding to a Ph.D. degree under the supervision of Prof. Sung Ju Hwang.

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	<ul style="list-style-type: none"> • Boeing Undergraduate Scholarship • KAIST Presidential Fellowship (KPF) • National Science and Engineering Scholarship 	Feb. 2018 - Aug. 2019 Mar. 2017 - Aug. 2019 Mar. 2015 - Feb. 2019
SKILLS	<ul style="list-style-type: none"> • Fluent in English • Fluent in Python and PyTorch 	
REFERENCES	<ul style="list-style-type: none"> • Prof. Sung Ju Hwang, Professor, KAIST <i>E-mail:</i> sjhwang82@kaist.ac.kr 	