

# JAEHYEONG JO

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## RESEARCH INTERESTS

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My research interest mainly focuses on understanding physical systems through the lens of graph-structured data and its geometric symmetries. In particular, I've been focusing on the generation of the graph with diffusion models and its applications to real-world tasks, for example, drug discovery or protein design.

## PUBLICATIONS

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### **Graph Generation with Destination-Driven Diffusion Mixture**

Jaehyeong Jo\*, Dongki Kim\*, and Sung Ju Hwang

Preprint, arXiv:2302.03596

### **Exploring Chemical Space with Score-based Out-of-distribution Generation**

Seul Lee, Jaehyeong Jo, and Sung Ju Hwang

Preprint, arXiv:2206.07632

### **Score-based Generative Modeling of Graphs via the System of Stochastic Differential Equations**

Jaehyeong Jo\*, Seul Lee\*, and Sung Ju Hwang

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

Neural Information Processing Systems (NeurIPS), 2021

\* denotes equal contribution.

## RESEARCH EXPERIENCE

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### **MLAI (Machine Learning & Artificial Intelligence) Lab, KAIST**

Seoul, Korea

Research Assistant (Advisor: Prof. Sung Ju Hwang)

Sep. 2021 - Present

- Conducting research on graph generative model with applications to drug discovery.

### **Kimlab, UofT**

Toronto, Canada

Visiting student (Host: Prof. Philip Kim)

Feb. 2023 - Feb. 2023

- Conducting research on protein generative model with diffusion models.

### **PAI (Probability Artificial Intelligence) Lab, KAIST**

Daejeon, Korea

Research Assistant (Advisor: Prof. Ganguk Hwang)

Mar. 2020 - Aug. 2021

- Conducted research on graphs (edge representation learning using hypergraph structure).

## TALKS

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### **Generation of Graph-Structured Data with Diffusion Models**

Toronto, Canada

in University of Toronto (UofT)

Feb 2023

### **Score-based Generative Modeling of Graphs via the SDEs**

Online

in LoGaG: Learning on Graphs and Geometry Reading Group

Oct. 2022

### **Learning with Graph Structure Data**

Pohang, Korea

in Pohang University of Science and Technology (POSTECH)

July 2022

**Score-based Graph Generation for Material Design**  
in Samsung Advanced Institute of Technology (SAIT)

Suwon, Korea  
Jun. 2022

## EDUCATION

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**Korea Advanced Institute of Science and Technology (KAIST)**

Ph.D. in Artificial Intelligence

Advisor: Proffesor Sung Ju Hwang

Seoul, Korea  
Sep. 2021 - Present

**Korea Advanced Institute of Science and Technology (KAIST)**

M.S. in Mathematical Sciences

Advisor: Professor Ganguk Hwang

Daejeon, Korea  
Mar. 2020 - Aug. 2021

**Korea Advanced Institute of Science and Technology (KAIST)**

B.S. in Mathematical Sciences

Minor in Computer Science & Engineering

GPA: 3.75/4.3

Daejeon, Korea  
Mar. 2016 - Feb. 2020

## ACADEMIC SERVICES

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### Conference Reviewers

- Learning on Graphs Conference (LoG), 2022
- Conference on Neural Information Processing Systems (**NeurIPS**), 2022
- International Conference on Machine Learning (**ICML**), 2022