

# YUNHUI JANG

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## RESEARCH INTEREST

My research goal is to build generative models for structured data. Specifically, I focus on graph generative models, molecular generative models, AI4Science, etc. My previous research focused on

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|--|------------------------------------|
| • AI4Science:                            | C1, C2, C3, C4, C5, C6, C8, P1, P2 |
| • Large language models for science:     | C5, C6, C8, P1, P2                 |
| • Generative models for structural data: | C1, C2, C4                         |

## WORK EXPERIENCE

<b>Valence Labs</b> , Research intern, (Manager: Emmanuel Noutahi)	Montreal, Canada / Jul 2025 - Dec 2025
• Conducted research on constructing LLM agent for reasoning and developing reasoning models for virtual cells	
<b>Netmarble</b> , Research intern	Seoul, South Korea / Jul 2018 - Aug 2018
• RNN-based anomaly detection	
<b>JoyCity</b> , Intern	Seoul, South Korea / Jun 2017 - Aug 2017
• Data analysis on marketing KPIs	

## EDUCATION

<b>KAIST</b> , Ph.D. student in Graduate School of AI (advisor: Prof. Sungsoo Ahn)	Feb 2025 - Aug 2027 (expected)
<b>POSTECH</b> , M.S. in Graduate School of AI (advisor: Prof. Sungsoo Ahn)	Sep 2022 - Feb 2025
<b>RWTH</b> , Exchange student in Computer Science	Mar 2019 - Feb 2020
<b>POSTECH</b> , B.S. in Industrial & Management Engineering - cum laude	Mar 2015 - Aug 2020

## PUBLICATIONS

C: conference, J: journal, W: workshop, P: preprint / \* equal contribution

- [P2] INDIBATOR: Diverse and Fact-Grounded Individuality for Multi-Agent Debate in Molecular Discovery  
Yunhui Jang, Seonghyun Park, Jaehyung Kim, Sungsoo Ahn
- [P1] Can LLMs Generate Diverse Molecules? Towards Alignment with Structural Diversity  
Hyosoon Jang, Yunhui Jang, Jaehyung Kim, Sungsoo Ahn
- [C8] Improving Chemical Understanding of LLMs via SMILES Parsing  
Yunhui Jang, Jaehyung Kim, Sungsoo Ahn  
*Conference on Empirical Methods in Natural Language Processing (EMNLP) (Main), 2025*
- [C7] Self-Training Large Language Models with Confident Reasoning  
Hyosoon Jang, Yunhui Jang, Sungjae Lee, Jungseul Ok, Sungsoo Ahn  
*Conference on Empirical Methods in Natural Language Processing (EMNLP) (Findings), 2025*
- [C6] MT-MOL: Multi Agent System with Tool-based Reasoning for Molecular Optimization  
Hyomin Kim, Yunhui Jang, Sungsoo Ahn  
*Conference on Empirical Methods in Natural Language Processing (EMNLP) (Findings), 2025*
- [C5] Structural Reasoning Improves Molecular Understanding of LLM  
Yunhui Jang, Jaehyung Kim, Sungsoo Ahn  
*Annual Meeting of the Association for Computational Linguistics (ACL) (Main), 2025*  
*NeurIPS AIDrugX Workshop, 2024*
- [C4] Pessimistic Backward Policy for GFlowNets  
Hyosoon Jang, Yunhui Jang, Minsu Kim, Jinkyoo Park, Sungsoo Ahn  
*Conference on Neural Information Processing Systems (NeurIPS), 2024*

[C3] Hybrid neural representations for spherical data  
Hyomin Kim, Yunhui Jang, Jaeho Lee, Sungsoo Ahn  
*International Conference on Machine Learning (ICML), 2024*

[C2] A simple and scalable representation for graph generation  
Yunhui Jang, Seul Lee, Sungsoo Ahn  
*International Conference on Learning Representations (ICLR), 2024*  
*NeurIPS GLFrontiers Workshop, 2023*

[C1] Graph generation with  $K^2$ -trees  
Yunhui Jang, Dongwoo Kim, Sungsoo Ahn  
*International Conference on Learning Representations (ICLR), 2024*  
*ICML Structured Probabilistic Inference & Generative Modeling Workshop, 2023*  
**Bronze Prize in 30th Samsung Humantech Paper Awards**  
**Winner in 2024 Qualcomm Innovation Fellowship Korea**

## HONORS & AWARDS

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Research Subsidies for Ph.D. Candidates, NRF (\$40,000)	2025-present
Winner in Qualcomm Innovation Fellowship Korea, Qualcomm (\$3,000)	2024
Presidential Science Scholarship, South Korea (\$70,000)	2024-present
Travel Award, ICLR (\$1,500)	2024
Bronze Prize in 30th Samsung Humantech Paper Awards, Samsung, (\$4,000)	2023
POSTECHIAN Fellowship, POSTECH, (\$3,000)	2022, 2023
RWTH Aachen University Exchange Scholarship, RWTH Aachen, (\$3,900)	2019
Realize Your Dream Scholarship, Blizzard Entertainment, (\$2,500)	2018
Presidential Science Scholarship, South Korea, (\$16,000)	2015-2020

## SERVICES

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Conference Reviewer: NeurIPS 2023-2025, ICLR 2024-2026, ICML 2024-2025, AAAI 2025-2026

## TALKS

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<b>Improving Structural Understanding of Molecular LLMs</b>	
AI Alliance, AI in Materials & Chemistry Webinar Series	Aug 2025
LG AI research, Seoul	Jun 2025
<b>Graph Generation with <math>K^2</math>-trees</b> , Qualcomm, Seoul	Mar 2025
<b>Speaking the Structure: Generative Models in Molecular Science</b> , MILA, Montreal	Dec 2024

## TEACHING

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<b>Teaching Assistant</b> , POSTECH, CSED105: Introduction to AI	Sep 2023 - Dec 2023
<b>Teaching Assistant</b> , LAIDD, Introduction to Geometric deep learning	Oct 2023 - Nov 2023
<b>Teaching Assistant</b> , POSTECH, CSED490B: Introduction to machine learning	Sep 2022 - Dec 2022
<b>Teaching Assistant</b> , Hyundai Steel, AI expert course	Oct 2022 - Nov 2022