

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

- 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

- Valence Labs**, 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
- Netmarble**, Research intern Seoul, South Korea / Jul 2018 - Aug 2018
- RNN-based anomaly detection
- JoyCity**, Intern Seoul, South Korea / Jun 2017 - Aug 2017
- Data analysis on marketing KPIs

EDUCATION

- KAIST**, Ph.D. student in Graduate School of AI (advisor: Prof. Sungsoo Ahn) Feb 2025 - Aug 2027 (expected)
- POSTECH**, M.S. in Graduate School of AI (advisor: Prof. Sungsoo Ahn) Sep 2022 - Feb 2025
- RWTH**, Exchange student in Computer Science Mar 2019 - Feb 2020
- POSTECH**, 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

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

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

TALKS

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

TEACHING

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