

Nayoung Kim

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Education

Ph.D. Korea Advanced Institute of Science and Technology (KAIST), Graduate School of Artificial Intelligence	Seoul, South Korea Feb 2025 – present
• Advisor: Sungsoo Ahn	
M.S. Korea Advanced Institute of Science and Technology (KAIST), Graduate School of Artificial Intelligence	Daejeon, South Korea Feb 2022 – Aug 2024
• Advisor: Jinkyoo Park	
B.S. Korea Advanced Institute of Science and Technology (KAIST), Chemical and Biomolecular Engineering	Daejeon, South Korea Aug 2017 – Feb 2022
• GPA: 4.14/4.30 (Summa Cum Laude)	

Experience

Pohang University of Science and Technology (POSTECH) , Researcher	Pohang, South Korea Sept 2024 – Jan 2025
• Advisor: Sungsoo Ahn	
• Topic: Generative model for metal-organic frameworks	
Korea Advanced Institute of Science and Technology (KAIST) , M.S	Daejeon, South Korea Feb 2022 – Aug 2022
• Advisor: Jay Hyung Lee	
• Topic: Thermodynamic and kinetic modeling of electric vacuum swing adsorption (EVSA) cycle for efficient direct air capture (DAC)	
Korea Advanced Institute of Science and Technology (KAIST) , Research Intern	Daejeon, South Korea June 2021 – Aug 2021
• Advisor: Jay Hyung Lee	
• Topic: Modeling polarization in electrochemical processes	
Korea Advanced Institute of Science and Technology (KAIST) , Research Intern	Daejeon, South Korea Dec 2020 – Feb 2021
• Advisor: Jinwoo Lee	
• Topic: Analyzing mechanism of potassium-ion batteries (KIB)	
• Topic: Intercalation-conversion hybrid cathode using V5S8 in lithium-sulfur battery to improve energy density	
SK Hynix , Intern	Icheon, South Korea Dec 2019 – Feb 2020
• Topic: Modeling the relationship between zone 1 and zone 2 in CMP head for accurate prediction of removal rate (Excellence Award)	

Publications

Flexible MOF Generation with Torsion-Aware Flow Matching	2025
Nayoung Kim, Seongsu Kim, Sungsoo Ahn	
arxiv.org/abs/2505.17914 (NeurIPS)	
High-order Equivariant Flow Matching for Density Functional Theory Hamiltonian Prediction	2025
Seongsu Kim, Nayoung Kim, Sungsoo Ahn	
arxiv.org/abs/2505.18817 (NeurIPS)	
Spotlight Presentation (688/21575=3.19%)	
MOFFlow: Flow Matching for Structure Prediction of Metal-Organic Frameworks	2025
Nayoung Kim, Seongsu Kim, Minsu Kim, Jinkyoo Park, Sungsoo Ahn	

arxiv.org/abs/2410.17270 (ICLR, NeurIPS AIDrugX Workshop)

Decoupled Sequence and Structure Generation for Realistic Antibody Design

2025

Nayoung Kim, Minsu Kim, Sungsoo Ahn, Jinkyoo Park

arxiv.org/abs/2402.05982 (TMLR)

Awards & Honors

Korea National Research Foundation (NRF) Ph.D. Fellowship

Sept 2025 – Aug 2027

SK Hynix Internship Excellence Award

Feb 2021

Korea National Science & Technology Scholarship

2019 – 2021

Awarded in Fall 2019, Spring 2020, Fall 2020, and Spring 2021

Dean's List of College of Engineering, KAIST

2019 – 2021

Awarded in Spring 2019, Fall 2019, and Spring 2021

Academic Excellence Scholarship of Chemical and Biomolecular Engineering, KAIST

2019 – 2020

Awarded in Spring 2019 and Fall 2020

Projects

Deep Generative Models for Simulation and Design of Metal-Organic Frameworks

Mar 2025 – Sept 2025

NVIDIA Academic Grant Program Award

Talks

MOFFlow: Flow Matching for Structure Prediction of Metal-Organic Frameworks

Nov 2024

KAIST-MILA Prefrontal AI Research Center

Reviewer

Conference

ICLR 2025, NeurIPS 2025, ICLR 2026

Skills

Languages: Korean (native), English (fluent), Chinese (basic)