

Nayoung Kim

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Education

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|---|---|
| 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

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|---|--|
| 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

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| 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

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

SK Hynix Internship Excellence Award

Feb 2021

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)