

Younghun Kim | Curriculum Vitae

Korea Advanced Institute of Science & Technology
Graduate Researcher, Dept. of Chemical and Biomolecular Engineering
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Education

KAIST (Korea Advanced Institute of Science and Technology) — Daejeon, Korea

Ph.D. Candidate, Department of Chemical and Biomolecular Engineering (Sep 2023 - Aug 2027, Expected)

Advisor: Jihan Kim

KAIST (Korea Advanced Institute of Science and Technology) — Daejeon, Korea

M.S., Department of Chemical and Biomolecular Engineering (Sep 2021 - Aug 2023)

Advisor: Jihan Kim

Case Western Reserve University — Cleveland, OH, USA

B.S., Department of Chemical Engineering (Sep 2015 - Aug 2021)

Research Expertise

AI-Based Material Design

- Inverse-design frameworks integrating machine learning and Genetic Algorithms (GA) for MOFs
- Quantum computing algorithms and Hamiltonian modeling for combinatorial optimization

Data-Driven Discovery and Materials Informatics

- High-throughput simulation database construction and ML modeling using using RDKit descriptors and Morgan fingerprints
- Automated text-mining and data extraction pipelines utilizing LLM agents
- Data-driven performance prediction models for MOF property prediction and lithium metal batteries

Molecular Simulation and Mechanistic Studies of Materials

- GCMC simulation for molecular adsorption and Henry's Coefficient calculations
- DFT simulations for Nudged Elastic Band (NEB) calculations and free energy evaluation for thermodynamic and kinetic evaluation of gas separation mechanisms

- Molecular dynamic simulations for transport behavior analysis and integration of Reactive Force Field (ReaxFF) via LAMMPS for thermal amorphization and melt-quenching simulations
- Machine Learning Interatomic Potentials (MLIP) for screening CO₂ Direct Air Capture (DAC) candidate materials with high fidelity

Technical Skills

- **Programming & Data Science:** Python, PyTorch, Scikit-learn, Pandas, Matplotlib, RDKit, Shell script
- **Molecular Simulation:** VASP, RASPA, LAMMPS, Gaussian, ASE, Pymatgen, Machine Learning Interatomic Potentials (MLIP)
- **Quantum Computing & Generative AI:** IBM Qiskit, Large Language Models (LLM agents, Data Mining)

Publications

(2026)

[1] **Y. Kim**, D. Kim, S.Kim, Y. Lim, J.Kim*. "Framework-Templated Gas Lattices in Metal-Organic Frameworks." Nature Communications.

[2] S. Han, T. Bae, J.Kim, **Y. Kim**, J. Kim*. "Large Language Models for Porous Materials: From Text Mining to Autonomous Laboratory." Digital Discovery.

[3] J.Lee, J.Woo, **Y.Kim**, S. Kim, C. Paulina, H. Park, H. T. Kim*, S. Park*, J.Kim*. "LLMB: AI agent for lithium metal battery research using large language model." ACS Central Science.

(2025)

[4] Y. Jeong, **Y. Kim**, W.S. Jeong, H. Choi, J. Kim*, T. Bae*. "Nitrogen-enriched porous organic polymers for high-performance CO₂/N₂ separation in mixed-matrix membranes." Journal of Membrane Science.

[5] S.Kang, **Y. Kim**, J.Kim*. "Quantum Computing-Based Design of Multivariate Porous Materials." ACS Central Science. *Co-First Author

[6] **Y. Kim**, W. Lee, J.Kim*. "Amorphous Metal-Organic Framework Database for Amorphization Prediction and CO₂ Direct Air Capture Screening." ACS Applied Materials & Interfaces.

Awards & Honors

- **Best Oral Presentation Award** (Apr 2026) — KIChE (The Korean Institute of Chemical Engineers) Spring Meeting
- **Term Honor: Dean's High Honors** (May 2020) — Case Western Reserve University
- **Term Honor: Dean's High Honors** (Dec 2019) — Case Western Reserve University
- **Term Honor: Dean's Honor List** (Dec 2018) — Case Western Reserve University

References

Jihan Kim

Professor, Department of Chemical and Biomolecular Engineering, KAIST

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