

Honghui Kim

Postdoctoral Researcher, KAIST Graduate School of AI

ildmb96@kaist.ac.kr [Google Scholar](#) [GitHub](#) [LinkedIn](#) honghuikim.github.io

I work at the interface of **machine learning**, **computational chemistry**, and **experiment** to accelerate real-world materials discovery.

RESEARCH EXPERIENCE

2026.03–Present Daejeon, Korea	Postdoctoral Researcher KAIST Graduate School of AI Advisor: Prof. Sungsoo Ahn
2020.02–2026.02 Daejeon, Korea	Graduate Student Researcher KAIST Advisor: Prof. Jihan Kim
2023.04–2023.10 Atlanta, GA	Visiting Researcher Georgia Institute of Technology Advisor: Prof. Andrew J. Medford

EDUCATION

2022.03–2026.02 Daejeon, Korea	Ph.D., Chemical and Biomolecular Engineering KAIST Advisor: Prof. Jihan Kim. Dissertation: <i>Closing the Simulation–Experiment Gap in Metal–Organic Frameworks: Computational Methodology and Structural Data Reliability.</i>
2020.03–2022.02 Daejeon, Korea	M.S., Chemical and Biomolecular Engineering KAIST Advisor: Prof. Jihan Kim.
2015.03–2020.02 Daejeon, Korea	B.S., Chemical and Biomolecular Engineering KAIST Cum Laude.
2018.09–2019.02 Dortmund, Germany	Exchange Student TU Dortmund

SELECTED PUBLICATIONS

2026 Preprint	MADField: Multi-fidelity Amortized Density Field for Adsorption in Nanoporous Materials Y. Kim, S. Kim, S. Ahn*, & H. Kim* . arXiv:2606.21284
2025 Preprint	LitMOF: An LLM Multi-Agent for Literature-Validated Metal–Organic Frameworks Database Correction and Expansion H. Kim , D. Kim, & J. Kim*. arXiv:2512.01693
2024 J. Phys. Chem. C	Assessing Exchange–Correlation Functionals for Heterogeneous Catalysis of Nitrogen Species H. Kim , N. K. Yu, N. Tian, & A. J. Medford*. doi:10.1021/acs.jpcc.4c01497
2024 Adv. Mater.	Boosting Alkaline Hydrogen Oxidation Activity of Ru Single-Atom through Promoting Hydroxyl Adsorption on Ru/WC_{1–x} Interfaces J. Park [†] , H. Kim[†] , S. Kim, S. Y. Yi, H. Min, D. Choi, S. Lee, J. Kim*, & J. Lee*. doi:10.1002/adma.202308899
2022 RSC Advances	Theoretical Study of Induced Selective N₂ Binding under an Electric Field in MOF-74: Application for N₂/CH₄ Separations H. Kim & J. Kim*. doi:10.1039/D2RA04216A

FULL PUBLICATION LIST

Journal Articles

- 2025
ACS Nano
Photothermal Annealing-Enabled Millisecond Synthesis of Carbon Nanooxions and Simultaneous Single-Atom Functionalization.
D. Jeon, H. Shin, J. H. Cha, **H. Kim**, S. Park, J. Ahn, S. H. Cho, C. Park, D. H. Kim, E. Shin, H. Baik, J. Kim, S. Y. Choi*, & I. D. Kim*. doi:10.1021/acsnano.5c11229
- 2024
JACS Au
From Data to Discovery: Recent Trends of Machine Learning in Metal–Organic Frameworks.
J. Park, **H. Kim**, Y. Kang, Y. Lim, & J. Kim*. doi:10.1021/jacsau.4c00618
- 2024
J. Phys. Chem. C
Assessing Exchange–Correlation Functionals for Heterogeneous Catalysis of Nitrogen Species.
H. Kim, N. K. Yu, N. Tian, & A. J. Medford*. doi:10.1021/acs.jpcc.4c01497
- 2024
Adv. Mater.
Boosting Alkaline Hydrogen Oxidation Activity of Ru Single-Atom through Promoting Hydroxyl Adsorption on Ru/WC_{1-x} Interfaces.
J. Park†, **H. Kim**†, S. Kim, S. Y. Yi, H. Min, D. Choi, S. Lee, J. Kim*, & J. Lee*. doi:10.1002/adma.202308899
- 2023
ACS Sensors
Computational Prediction of Stacking Mode in Conductive Two-Dimensional Metal–Organic Frameworks.
M. Jeon, M. Kim, J. S. Lee, **H. Kim**, S. J. Choi, H. R. Moon, & J. Kim*. doi:10.1021/acssensors.3c00715
- 2023
Adv. Funct. Mater.
Imparting Metal Oxides with High Sensitivity toward Light-Activated NO₂ Detection via Tailored Interfacial Chemistry.
S. Park, S. H. Jeon, **H. Kim**, J. Philips, D. H. Oh, J. Ahn, M. Kim, C. Park, S. Hong, J. Kim, W. C. Jung, & I. D. Kim*. doi:10.1002/adfm.202214008
- 2022
RSC Advances
Theoretical Study of Induced Selective N₂ Binding under an Electric Field in MOF-74: Application for N₂/CH₄ Separations.
H. Kim & J. Kim*. doi:10.1039/D2RA04216A

Conference Papers

- 2026
ICML
Machine Learning Hamiltonians are Accurate Energy-Force Predictors.
S. Kim, C. Lee, Y. Kim, S. Yun, **H. Kim**, N. Kim, C. Park, S. Han, S. Lim*, & S. Ahn*. arXiv:2602.16897
- 2026
ICML
CatFlow: Co-generation of Slab-Adsorbate Systems via Flow Matching.
M. Kim, N. Kim, **H. Kim**, & S. Ahn*. arXiv:2602.05372

Preprints

- 2026
MADField: Multi-fidelity Amortized Density Field for Adsorption in Nanoporous Materials.
Y. Kim, S. Kim, S. Ahn*, & **H. Kim***. arXiv:2606.21284
- 2026
AtomMOF: All-Atom Flow Matching for MOF-Adsorbate Structure Prediction.
N. Kim, **H. Kim**, S. Yu, M. Kim, S. Kim, & S. Ahn*. arXiv:2602.07351
- 2026
A Systematic Evaluation of Co-folding Model Representations for Small-Molecule Learning.
H. Jang, H. Seo, **H. Kim**, S. Park, T. Kim, Y. Jang, & S. Ahn*. arXiv:2602.13249
- 2025
LitMOF: An LLM Multi-Agent for Literature-Validated Metal–Organic Frameworks Database Correction and Expansion.
H. Kim, D. Kim, & J. Kim*. arXiv:2512.01693

†equal contribution, *corresponding author

PRESENTATIONS

- Oral
MRS Fall 2025, “LLM-Driven Multi-Agent Curation and Expansion of Metal–Organic Frameworks Database”. Boston, MA. Dec 2025.
- Oral
KICHe Fall Meeting and International Symposium, “LLM-Driven Multi-Agent Curation and Expansion of Metal–Organic Frameworks Database”. Jeju, Korea. Oct 2025.

Poster	KIChE Fall Meeting and International Symposium, "Induced Selective N ₂ Binding under Electric Field: Application for the Separation of N ₂ /CH ₄ and N ₂ /CO ₂ ". Gwangju, Korea. Oct 2021.
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SKILLS

Computational	Python (PyTorch, LangGraph, LangChain), VASP (DFT), Gaussian (DFT), LAMMPS (MD), RASPA (GCMC)
Language	English, Korean

HONORS & AWARDS

2018	Mirae Asset Global Exchange Scholarship
2015 - 2025	KAIST Support Scholarship