

# Huiwon Jang

Postdoctoral Associate

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## Research Experience

**Postdoctoral Associate, Massachusetts Institute of Technology (MIT), March, 2026 – Present.**

- Advisor: Prof. Heather J. Kulik

## Education

**Ph.D. Korea Advanced Institute of Science and Technology (KAIST), Feb. 2022 – Feb. 2026**

- Advisor: Prof. Jihan Kim
- Thesis: Accelerating Material Discovery for Metal–Organic Frameworks and Mixed Matrix Membranes Using Machine Learning and Molecular Simulation.

**M.S. Korea Advanced Institute of Science and Technology (KAIST), Mar. 2020 – Feb. 2022**

- Advisor: Prof. Jihan Kim
- Thesis: Machine Learning based Epoxy Resins Properties Prediction

**B.S. Korea Advanced Institute of Science and Technology (KAIST), Mar. 2015 – Feb. 2020**

- Advisor: Prof. Jihan Kim
- Thesis: Blockchain based Plastic Recycling

## Research Interests

### 1. Accelerated Materials Discovery

- Implement high-throughput virtual screening (HTVS) integrated with data-driven methods and multi-scale simulations to accelerate the discovery of materials. Research focuses on metal-organic frameworks (MOFs), mixed matrix membranes (MMMs), and polymers.

### 2. Multi-scale Simulations

- Employ molecular simulations across multiple scales, including DFT, MD, and GCMC to model complex material behaviors and properties. Each method is strategically applied to balance accuracy and computational efficiency, providing chemical insights and high-fidelity data for materials discovery.

### 3. Data-driven methods & Large Language Models (LLMs)

- Develop machine learning models to predict material properties and screen promising candidates. Incorporating LLMs into computational workflows enables large-scale data extraction and the development of autonomous research pipelines, significantly enhancing the speed of materials discovery.

### 4. Metal-organic frameworks (MOFs)

- MOFs exhibit a vast design space with high tunability, which highlights the efficiency of computational strategies to identify promising candidates. Key applications include gas separation, carbon capture, and gas storage.

## Publications

7. C. Paulina<sup>‡</sup>, D. Son<sup>‡</sup>, **H. Jang<sup>‡</sup>**, H. Park, J. Kim, J. Lee, S. Park<sup>\*</sup>, “Addressing Low E/S and N/P Ratio Challenges in Li–S Batteries with a Multifunctional Interlayer”, *Small*, e08573, **2026**

6. H. Park, J. W. Baek, **H. Jang**, H. Shin, J. Kim, I. Kim\*, “Defect-Mediated In Situ CNT Growth in Hollow Porous Carbon From ZIF-8/ZIF-67 Bilayers for Efficient and Stable ORR Catalysis”, *Small*, 22(4), e09739, **2026**
5. **H. Jang**, J. Kim\*, “Computational Screening and Analysis of Compatibility in Mixed Matrix Membranes for Enhanced Gas Separation”, *Separation and Purification Technology*, 134852, **2025**
4. W. Lee, Y. Kang, T. Bae, **H. Jang**, S. Han, J. Kim\*, “Harnessing Large Language Model to Collect and Analyze Metal-organic Framework”, *Journal of the American Chemical Society*, 147(5), 3943-3958. **2025**.
3. **H. Jang**, D. Ryu, W. Lee, G. Park, J. Kim\*, “Machine Learning based Epoxy Resins Properties Prediction”, *Molecular Systems Design & Engineering*, 9(9), 959-968, **2024**.
2. J. Shin, G. Lee, M. Choi, **H. Jang**, Y. Lim, G. S. Kim, S. H. Nam, S. H. Baek, H. C. Song, J. Kim, C. Y. Kang, J. O. Lee, S. Jeon, D. Cho, J. S. Jang\*, “Atomically mixed catalysts on a 3D thin-shell TiO<sub>2</sub> for dual-modal chemical detection and neutralization”, *Journal of Materials Chemistry A*, vol. 11, 18195, **2023**.
1. C.K. Chang, H.J. Yu, **H. Jang**, T.H. Hung, C.K. Chang, J. Kim\*, J.S. Lee\*, D.Y. Kang\* , “Conformational-change-induced selectivity enhancement of CAU-10-PDC membrane for H<sub>2</sub>/CH<sub>4</sub> and CO<sub>2</sub>/CH<sub>4</sub> separation”, *Journal of Membrane Science Letters*, vol. 1, 10005, **2021**.

## Presentations

7. Centre Européen de Calcul Atomique et Moléculaire (July, **2025**)
  - Machine Learning Framework for Predicting Gas Separation Performance and Interfacial Compatibility in Mixed Matrix Membranes, Poster Presentation
6. KAIST-MIT Future Energy Initiative Symposium (Dec, **2024**)
  - Data-driven Approach for Next-Generation Battery using Large Language Models, Oral Presentation
5. International Symposium on Chemical Engineering, ISChE (Nov, **2024**)
  - Enhancing Mixed Matrix Membrane Performance through Compatibility Analysis, Oral Presentation
4. The Korean Institute of Chemical Engineers (Oct, **2024**)
  - Enhancing Mixed Matrix Membrane Performance through Compatibility Analysis, Oral Presentation
3. The Korean Institute of Chemical Engineers (Apr, **2023**)
  - “Machine Learning based Epoxy Resins Properties Prediction, Oral Presentation
2. The International Conference on Electronic Materials and Nanotechnology for Green Environment, ENGE (Nov, **2022**)
  - Machine Learning based Epoxy Resins Properties Prediction, Poster Presentation
1. 2019 Winter/Spring semester URP (Undergraduate Research Program) (July, **2019**)
  - Blockchain based Plastic Recycling, Oral and Poster Presentation

## Skill Highlights

- **Molecular Simulation Tools:** LAMMPS, Gaussian, VASP, GCMC
- **Machine Learning Tools:** Scikit-learn
- **Large Language Models**
- **Programming Language:** Python
- **Visualization Tools:** Material Studio, VMD, Avogadro, VESTA, OVITO