

Junkil Park | Curriculum Vitae

Seoul National University

Postdoctoral Researcher, Department of Chemical and Biological Engineering

E-mail: junkil0617@gmail.com / junkil0617@snu.ac.kr

Education

Korea Advanced Institute of Science and Technology (KAIST) Daejeon, Korea
Ph.D. Department of Chemical and Biomolecular Engineering 2021-2024
Advisor: Jihan Kim (jihankim@kaist.ac.kr)

Korea Advanced Institute of Science and Technology (KAIST) Daejeon, Korea
M.S. Department of Chemical and Biomolecular Engineering 2019-2021
Advisor: Jihan Kim (jihankim@kaist.ac.kr)

Korea Advanced Institute of Science and Technology (KAIST) Daejeon, Korea
B.S. Department of Chemical and Biomolecular Engineering 2015-2018

Research Experience

Imperial College London London, United Kingdom
Research Associate 2026-
Advisor: Aron Walsh (a.walsh@imperial.ac.uk)

Seoul National University (SNU) Seoul, Korea
Postdoctoral Researcher 2024-
Advisor: Yousung Jung (yousung.jung@snu.ac.kr)

Northwestern University Evanston, IL, USA
Visiting Scholar 2022-2023
Advisor: Randall. Q. Snurr (snurr@northwestern.edu)

Research Interest

Artificial Intelligence, Materials Inverse Design, Generative Models, Molecular Simulation

Deployed Projects

- **ChargeDIFF** ([link](#))

ChargeDIFF is a generative model for inorganic materials that, for the first time, explicitly incorporates electronic structure information during the generation process. This deeper understanding of the material's chemical nature leads to improved generation performance.

- **MOFFUSION** ([link](#))

MOFFUSION is a multi-modal generative model for the design of metal-organic frameworks (MOFs). It leverages signed distance functions (SDFs) to represent structures and supports conditional generation on diverse modalities of data.

- **ZeoDIFF** ([link](#))

ZeoDIFF is the diffusion model for zeolite generation, representing the first application of diffusion models for the generation of porous materials. The framework for zeolite structure generation was developed by drawing inspiration from advances in image generation.

- **Amorphous PPN Database** ([link](#))

The first porous polymer network (PPN) database that accounts for their intrinsic amorphous nature through large-scale molecular dynamics (MD) simulations.

- **Genetic Algorithm for MOFs** ([link](#))

A genetic algorithm platform for MOFs, targeting structures with high hydrogen working capacities under cryogenic conditions.

Publications

First/Co-First author marked as *

2025

#15. Choi, J., Kim, S., **Park, J.**, Choi, J., An, S., and Jung, Y. Next-Generation AI for Accelerated Materials Discovery. (submitted)

#14. Kim, S., Choi, J., Jang, K., **Park, J.**, Bernales, V., Aspuru-Guzik, A., and Jung, Y. Materealize: a multi-agent deliberation system for end-to-end material design and synthesis. (submitted)

#13. **Park, J.***, Choi, J., and Jung, Y. Learning electrons to generate materials. (submitted)

#12. **Park, J.***, Lee, Y., and Kim, J. Multi-modal conditional diffusion model using signed distance functions for metal-organic framework generation. *Nature Communications* 2025 16:34

2024

#11. **Park, J.***, Lee, W., and Kim, J. Large-Scale Construction and Analysis of Amorphous Porous Polymer Network Materials. *ACS App. Mater. Interfaces* 2024, 16, 57190-57199

#10. **Park, J.***, Kim, H., Kang, Y., Lim, Y., and Kim, J. From Data to Discovery: Recent Trends of Machine Learning in Metal-Organic Frameworks. *JACS Au* 2024, 4, 3727-3743

#9. Hyun, T., **Park, J.***, So, J., Kim, J., and Koh, D. Unexpected molecular sieving of xylene isomers in polymer-metal-organic frameworks (PolyMOF) materials. *Advanced Science* 2024, 11, 2402980

#8. **Park, J.***, Gill, APS., Moosavi, SM., and Kim, J. Inverse design of porous materials: a diffusion model approach. *Journal of Materials Chemistry A* 2024, 12, 6507-6514

#7. Ko, Y., **Park, J.**, Zhang, X., Kang, L., Pham T., Boureau V., Pham-Huu, C., Kim, J., Zhong, L., and Zuttel. All platinum group metal-free catalysts using in liquid fuel operated direct borohydride fuel cells. *ACS Appl. Energy Mater* 2024, 7, 2, 639-648

2023

#6. Lee, J., Lim, H., **Park, J.**^{*}, Kim, M., Jung, J., Kim, J., and Kim, I. Flouring-Rich Organic Framework to Boost Electrochemical Kinetics and Storage of K⁺ Ions for Potassium-Ion Battery. *Advanced Energy Materials*, 2023, 13, 2300442

#5. **Park, J.**^{*}, Lim, Y., Lee, S., and Kim, J. Computational Design of Metal-Organic Frameworks with Unprecedented High Hydrogen Working Capacity and High Synthesizability. *Chemistry of Materials* 2023, 35, 1, 9-16

2022

#4. Dodson, R.A., **Park, J.**, Kim, J., Cliffe, M.J., and Cohen, S.M. Tethering Effects in Oligomer-Based Metal-Organic Frameworks. *Inorganic Chemistry* 2022, 61, 31, 12284-12292

2021

#3. Lim, Y., **Park, J.**, Lee, S., and Kim, J. Finely tuned inverse design of metal-organic frameworks with user-desired Xe/Kr selectivity. *Journal of Materials Chemistry A* 2021, 9, 21175-21183

#2. Sarango-Ramirez, M.K., **Park, J.**, Kim, J., Yoshida, Y., Lim, D.W., and Kitagawa, H. Void Space versus Surface Functionalization for Proton Conduction in Metal-Organic Frameworks. *Angew. Chem. Int. Ed.* 2021, 60, 20173-20177

2020

#1. **Park, J.**^{*}, Suh, B.L., and Kim, J. Computational design of a photoresponsive metal-organic framework for post combustion carbon capture. *J. Phys. Chem. C* 2020, 124, 24, 13162-13167