

Yunsung Lim

Postdoctoral Research Fellow @ Research Institute of Advanced Materials, Seoul National University

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(Last updated: 19th October, 2025)

Professional experience

Research Institute of Advanced Materials @ Seoul National University (SNU)

BK21 Postdoctoral research fellow (Alternative military service – Technical research personnel)

Advisor: Prof. Dr. Seungwu Han

Seoul, KR

Sep. 2025 - Present

Imperial College London

Visiting researcher in Department of Materials

Advisor: Prof. Dr. Aron Walsh

London, UK

Jul. 2023 - Jan. 2024

Korea Advanced Institute of Science and Technology (KAIST)

Graduate research assistant

Advisor: Prof. Dr. Jihan Kim

Daejeon, KR

Mar. 2020 - Aug. 2025

SK Hynix

Internship program

Team: DRAM Photo

Icheon, KR

Dec. 2018 - Feb. 2019

Korea Advanced Institute of Science and Technology (KAIST)

Undergraduate research assistant

Advisor: Prof. Dr. Jihan Kim

Daejeon, KR

Jun. 2018 - Aug. 2018

Mar. 2019 - Aug. 2019

Education

Korea Advanced Institute of Science and Technology (KAIST)

Ph.D. in Chemical and Biomolecular Engineering

Dissertation: Efficient Computational Modeling of Metal-Organic Frameworks for Greenhouse Gas Reduction

Advisor: Prof. Dr. Jihan Kim

GPA: 4.16/4.3

Daejeon, KR

Mar. 2022 – Aug. 2025

Korea Advanced Institute of Science and Technology (KAIST)

M.S. in Chemical and Biomolecular Engineering

Thesis: Finely Tuned Inverse Design of Metal-Organic Frameworks for Selective Xenon Adsorption

Advisor: Prof. Dr. Jihan Kim

GPA: 4.17/4.3

Daejeon, KR

Mar. 2020 - Feb. 2022

Korea Advanced Institute of Science and Technology (KAIST)

B.S. in Chemical and Biomolecular Engineering

GPA: 4.07/4.3 (Rank: 2/74, Honors: Summa cum laude)

Daejeon, KR

Mar. 2016 - Feb. 2020

Research interests

- **Atomistic modeling:** Unraveling catalytic mechanisms (e.g Nitrogen reduction reaction (NRR), CO₂ reduction reaction (CO₂RR), or etc...) within the materials surface using the first-principle calculations and machine learning.
- **Data-driven materials design:** Construction of materials database and screening the constructed database *via* high-throughput virtual screening (HTVS) method to discover the candidates for the environmental and energy applications (e.g. Gas storage, Gas separation, Catalyst, Electrode, or etc...).
- **Material analysis:** In-depth molecular level simulation using various computational chemistry method to align with the experimental results and suggest underlying mechanism for the experimentally validated phenomenon.

Honors

- **Postdoctoral Researcher Fellowship of BK21 Plus Program**, SNU Materials Education/Research Division for Creative Global Leaders @ Seoul National University (SNU), Sep. 2025 – Aug. 2026
- **International Research Fellowship of BK21 Plus Program**, Program for Intelligent Multi-scale Chemical & Biomolecular Engineering @ Korea Advanced Institute of Science and Technology (KAIST), Jul. 2023 – Jan. 2024
- **Department Honors Scholarship**, Korea Advanced Institute of Science and Technology (KAIST), 2018 spring

Publications

(*: Corresponding author, ‡: Co-first author / 1st author: 6, Co-author: 10)

17. J. Kim[‡], J. You[‡], Y. Park, **Y. Lim**, Y. Kang, J. Kim, H. Jeon, D. Hong, S.Y. Lee, S. Choi, Y. Kim, J.W. Lee, S. Han^{*}, “Optimizing Cross-Domain Transfer for Universal Machine Learning Interatomic Potentials”, *arxiv*, 2025
16. **Y. Lim**, W. Jeong, H. Jung, H.L. Choi, T.-H. Bae, J.H. Lee^{*}, and J. Kim^{*}, “Tuning Pore Chemistry of Metal-Organic Frameworks using Anionic Pillars for Humid-tolerant CO₂ Capture”, *Chem. Mater.*, 37 (21), 8797-8808, 2025
15. K. Lee[‡], M. Kim[‡], Y. Kwon[‡], S. Park[‡], **Y. Lim**, D. Kwak, J. Jeong, B. Kim, J. Ahn, J. Kim, Y.-H. Cho, I.-D. Kim^{*} and I. Park^{*}, “Enabling Weather-Independent Gas Detection through Deep Learning on Light-Activated Sensors”, *ACS Nano*, 19 (44), 38327-38339, 2025
14. Y. Chiang, T. Kreiman, C. Zhang, M.C. Kuner, E.J. Weaver, I. Amin, H. Park, **Y. Lim**, J. Kim, D. Chrzan, A. Walsh, S.M. Blau, A.S. Krishnapriyan, M. Asta, “MLIP Arena: Advancing Fairness and Transparency in Machine Learning Interatomic Potentials via an Open, Accessible Benchmark Platform”, *NeurIPS 2025 Datasets and Benchmarks track (spotlight; top 3.5%)*, 2025
13. D. Kim, **Y. Lim**, and J. Kim^{*}, “Refining a Generic Force Field for Predicting Phase Transitions in Wine-Rack Metal-Organic Frameworks”, *J. Chem. Theory Comput.*, 21 (11), 5599-5607, 2025
12. **Y. Lim**[‡], H. Park[‡], A. Walsh^{*}, and J. Kim^{*}, “Accelerating CO₂ direct air capture screening for metal-organic frameworks with a transferable machine learning force field”, *Matter*, 8 (7), 102203, 2025
11. J. Park, H. Kim, Y. Kang, **Y. Lim**, and J. Kim^{*}, “From Data to Discovery: Recent Trends of Machine Learning in Metal-Organic Frameworks”, *JACS Au*, 4 (10), 3727-4743, 2024 (Perspective)
10. **Y. Lim**[‡], B. Kim[‡], and J. Kim^{*}, “Data-Driven Design of Flexible Metal-Organic Frameworks for Gas Storage”, *Chem. Mater.*, 36 (11), 5465-5473, 2024

9. S. Park[†], M. Kim[†], **Y. Lim**, D.H. Oh, J. Ahn, C. Park, S. Woo, W.C. Jung, J. Kim, and I.D. Kim*, “Dual-photosensitizer synergy empowers ambient light photoactivation of indium oxide for high-performance NO₂ sensing”, *Adv. Mater.*, 36 (24), 2313731, 2024
8. 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*, and J.S. Jang*, “Atomically mixed catalysts on a 3D thin-shell TiO₂ for dual-modal chemical detection and neutralization.”, *J. Mater. Chem. A*, 11 (34), 18195-18206, 2023
7. J. Ahn[†], S. Park[†], D.H. Oh, **Y. Lim**, J.S. Nam, J. Kim, W.C. Jung, and I.D. Kim*, “Rapid Joule Heating Synthesis of Oxide-Socketed High-Entropy Alloy Nanoparticles as CO₂ Conversion Catalysts.”, *ACS Nano*, 17 (13), 12188-12199, 2023
6. G.S. Kim[†], **Y. Lim**[†], J. Shin, J. Yim, S. Hur, H.C. Song, S.H. Baek, S.K. Kim, J. Kim*, C.Y. Kang*, and J.S. Jang*, “Breathable MOFs layer on atomically grown 2D SnS₂ for stable and selective surface activation”, *Adv. Sci.*, 10 (17), 2301002, 2023 (Back cover featured)
5. J. Park, **Y. Lim**, S. Lee, and J. Kim*, “Computational Design of Metal-Organic Frameworks with Unprecedented High Hydrogen Working Capacity and High Synthesizability”, *Chem. Mater.*, 35 (1), 9-16, 2023.
4. S. Park, **Y. Lim**, D.H. Oh, J. Ahn, C. Park, M. Kim, W.C. Jung, J. Kim, and I.D. Kim*, “Steering selectivity in detection of exhaled biomarkers over oxide nanofibers dispersed with noble metals”, *J. Mater. Chem. A*, 11 (7), 3535-3545, 2023.
3. J.S. Jang*, **Y. Lim**, H. Shin, J. Kim, and T.G. Yun*, “Bi-directional water-stream behavior on multifunctional membrane for simultaneous energy generation and water purification”, *Adv. Mater.*, 35 (7), 2209076, 2023.
2. **Y. Lim**, and J. Kim*, “Application of transfer learning to predict diffusion properties in metal-organic frameworks”, *Mol. Syst. Des. Eng.*, 7 (9), 1056-1064, 2022.
1. **Y. Lim**, J. Park, S. Lee, and J. Kim*, “Finely tuned inverse design of metal-organic frameworks with user-desired Xe/Kr selectivity”, *J. Mater. Chem. A*, 9 (37), 21175-21183, 2021.

Teaching

Korea Advanced Institute of Science and Technology (KAIST)

Teaching assistant

(Course: Chemical and Biomolecular Engineering Laboratory)

Daejeon, KR

Mar. 2023 - Jun. 2023

Korea Advanced Institute of Science and Technology (KAIST)

Teaching assistant

(Course: Molecular Engineering Laboratory)

Daejeon, KR

Sep. 2022 - Dec. 2022

Korea Advanced Institute of Science and Technology (KAIST)

Teaching assistant

(Course: Introduction to Numerical Methods for Chemical and Biomolecular Engineers)

Daejeon, KR

Sep. 2020 - Dec. 2020

Korea Advanced Institute of Science and Technology (KAIST)

Teaching assistant

(Course: Chemical and Biomolecular Engineering Analysis)

Daejeon, KR

Mar. 2018 - Jun. 2018

Skills

Molecular simulation tools – Vienna Ab initio Simulation Package (VASP), RASPA, LAMMPS

Visualizer – Materials Studio, VESTA, VMD, OVITO

