Yunsung **Lim**

PhD CANDIDATE @ DEPARTMENT OF CHEMICAL AND BIOMOLECULAR ENGINEERING, KAIST

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Professional experience

Imperial College London — **London, UK**
Visiting researcher in Department of Materials — *Jul. 2023 - Jan. 2024*
Advisor: Prof. Dr. Aron Walsh

Korea Advanced Institute of Science and Technology (KAIST) — **Daejeon, KR**
Graduate research assistant — *Mar. 2020 - Present*
Advisor: Prof. Dr. Jihan Kim

SK Hynix — **Icheon, KR**
Internship program — *Dec. 2018 - Feb. 2019*
Team: DRAM Photo

Korea Advanced Institute of Science and Technology (KAIST) — **Daejeon, KR**
Undergraduate research assistant — *Jun. 2018 - Aug. 2018*
Advisor: Prof. Dr. Jihan Kim — *Mar. 2019 - Aug. 2019*

Education

Korea Advanced Institute of Science and Technology (KAIST) — **Daejeon, KR**
Ph.D. in Chemical and Biomolecular Engineering — *Mar. 2022 - present*
Advisor: Prof. Dr. Jihan Kim
GPA: 4.16/4.3

Korea Advanced Institute of Science and Technology (KAIST) — **Daejeon, KR**
M.S. in Chemical and Biomolecular Engineering — *Mar. 2020 - Feb. 2022*
Thesis: Finely Tuned Inverse Design of Metal-Organic Frameworks for Selective Xenon Adsorption
Advisor: Prof. Dr. Jihan Kim
GPA: 4.17/4.3

Korea Advanced Institute of Science and Technology (KAIST) — **Daejeon, KR**
B.S. in Chemical and Biomolecular Engineering — *Mar. 2016 - Feb. 2020*
GPA: 4.07/4.3 (Honors: Summa cum laude)

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

- **International Research Fellowship of BK21 Plus Program**, *South Korea*, 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: 4, Co-author: 7)

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 NO_2 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 TiO_2 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 CO_2 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 SnS_2 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.

Scientific achievements

International Conferences	1. "Data-Driven Design of Adsorption Responsive Flexible Metal-Organic Frameworks", *ChemIndix2024 (Saudi Arabia)*, 26/11/2024 (Poster presentation)

Teaching

Korea Advanced Institute of Science and Technology (KAIST) **Daejeon, KR**
Teaching assistant *Mar. 2023 - Jun. 2023*
(Course: Chemical and Biomolecular Engineering Laboratory)

Korea Advanced Institute of Science and Technology (KAIST) **Daejeon, KR**
Teaching assistant *Sep. 2022 - Dec. 2022*
(Course: Molecular Engineering Laboratory)

Korea Advanced Institute of Science and Technology (KAIST) **Daejeon, KR**
Teaching assistant *Sep. 2020 - Dec. 2020*
(Course: Introduction to Numerical Methods for Chemical and Biomolecular Engineers)

Korea Advanced Institute of Science and Technology (KAIST) **Daejeon, KR**
Teaching assistant *Mar. 2018 - Jun. 2018*
(Course: Chemical and Biomolecular Engineering Analysis)

Skills

Molecular simulation tools – *Vienna Ab initio Simulation Package (VASP), RASPA, LAMMPS*
Visualizer – *Materials Studio, VESTA, VMD, OVITO*
Programming language – *Python*