

# Seokhyun Choung

 seokhyun-choung-635919174 |  s-choung |  schoung.com

Research Institute of Advanced Materials (RIAM)  
Department of Materials Science and Engineering, Seoul National University

## Profile

AI-native chemical engineer developing next-generation catalysts to combat climate change through computational design. Supported by the Sejong Science Fellowship (2026-2031), I combine **machine learning** (Distillation/Fine-tuning/Generative diffusion/Multiscale simulation) with **ab initio calculations** to discover efficient catalytic materials for sustainable chemical processes ([project page](#)).

## Experience

- **Seoul National University** 2024 - Present  
Senior Research Associate Seoul, South Korea
  - Multiscale simulation and machine learned interatomic potentials for catalyst and energy materials design

## Education


- **Pohang University of Science and Technology (POSTECH)** 2020 - 2024  
Ph.D. Chemical Engineering (advisor: Prof. Jeong Woo Han) Pohang, South Korea
  - Computational Catalysis for electrochemical/thermal catalyst design and reaction mechanism
- **Pohang University of Science and Technology (POSTECH)** 2016 - 2020  
B.Sc. Chemical Engineering Pohang, South Korea
  - Research Intern at Computational Catalysis and Emerging Materials Laboratory (J.W. Han's Lab)
  - Visiting Research Intern at Seoul National University, Chemical Engineering (2018 Fall)
  - Visiting Research Intern at Technical University of Denmark, Physics (2019 Fall)

## Fellowships & Grants

- **Sejong Science Fellowship (KRW 100M/yr, ~USD 70K/yr)** 2026 - 2031  
Independent research fellowship for early-career scientists National Research Foundation of Korea (NRF)
- **Soseon Foundation Scholarship (KRW 10M)** 2023  
Graduate research scholarship for outstanding STEM students Soseon Foundation
- **Soseon Foundation Scholarship (KRW 20M)** 2022  
Graduate research scholarship for outstanding STEM students Soseon Foundation

## Publications (15 first-author, 1 in revision, 3 submitted)

† Equal contribution, \* Corresponding author

- Submitted. [Oxidation-driven single-atom reconstruction on nitrides for robust photocatalytic biosynthesis](#). **Joule**, submitted. Oh, D., Kim, C. H., Seo, H., Chi, S., Kim, U., Choi, M., **Choung, S.**, Stratmann, L., Wang, Y., Hollmann, F., Han, J. W.\*, Park, C. B.\*, Jung, W.\* (2026).
- Submitted. [Elucidating the impact of molybdenum speciation on carburization dynamics over Mo/ZSM-5 in methane dehydroaromatization: A combined experimental and machine-learning interatomic potential study](#). **ACS Catalysis**, submitted. Roh, J., Pophali, A., Kim, T., **Choung, S.**, Lim, Y. H., Kim, K., Seok, G., Han, J. W., Kim, D. H. (2026).
- Submitted. **1st** [Phase-transformation-enabled linear junctions drive high-rate electrosynthesis of H<sub>2</sub>O<sub>2</sub>](#). submitted. Kim, H.†, **Choung, S.**†, Ma, R.†, Fu, Z., Han, J. W.\*, An, J.\*, Bu, Y.\* (2026).
- In review. [TiO<sub>2</sub>-facet-dependent reconstruction of Pt nanoparticles during CO oxidation](#). **Nature Communications**, in revision. Kim, J.†, Kim, Y.†, Oh D., **Choung, S.**, Lee H., Lee H., Lee E., Kim J., Yoon S.\*, Han J. W.\*, An K.\* (2026).
26. **1st** [High-performance gas sensors through predictive material design](#). **Nature Sensors**, accepted. Kim, G.†, Shin, H.†, **Choung, S.**†, D'Andria, M., Han, J. W.\*, Güntner, A. T.\* (2026).
25. **1st** [Hierarchical ceria nanoarchitecture enabling accelerated lattice oxygen dynamics for advanced redox reactions](#). **Nature Communications**, accepted. [ [Code](#)] (IF = 15.7). **Choung, S.**†, Kim, Y.†, Jang, M. G.†, Cho, G. H., Kang, D., Lee, T., Lee, D., Han, S., Seo, B., Park, W., Kim, M., Seo, O., Watanabe, T., Kumara, L. S. R., Matsumura, D., Kim, T. Y., Kim, J. H., Kim, J., Han, J. W.\* (2026).

24. **1st** Angular relational knowledge distillation of machine learning interatomic potentials for scalable catalyst exploration. **npj Computational Materials**, accepted. [[Code](#)] (IF = 11.9). Lim, H.<sup>†</sup>, **Choung, S.<sup>†</sup>**, Moon, J., Han, J. W.\* (2026).
23. **1st** Dynamic Hydroxyl Bridge Mechanism for Selective Ozone Evolution on Ni-Sb-SnO<sub>2</sub>. **Applied Catalysis B: Environment and Energy**, 391, 126646. (IF = 21.1). **Choung, S.<sup>†</sup>**, Kim, S.<sup>†</sup>, Lee, J., Cho, K.\* , Han, J. W.\* (2026).
22. **1st** CatAgent: Multi-Agent Orchestration for Electrocatalyst Discovery. **Workshop on AI for Accelerated Materials Design, ICLR 2026**. [[Code](#)]. **Choung, S.**, Kim, H., Kim, J., Han, J. W.\* (2026).
21. **1st** Understanding oxygen transfer on ceria with Pt single atoms for surface reaction. **Nature Communications**, 17, 298. [[Code](#)] (IF = 15.7). Choi, Y.<sup>†</sup>, **Choung, S.<sup>†</sup>**, Han, J.<sup>†</sup>, Hwang, J., Jin, H., Kim, Y., Kim, J., Park, J. Y.\* , Han, J. W.\* , Lee, H.\* (2026).
20. FORK: First-Order Relational Knowledge Distillation for Machine Learning Interatomic Potentials. **Workshop on AI for Accelerated Materials Design, NeurIPS 2025**. [[Code](#)]. Lim, H., **Choung, S.**, Han, J. W.\* (2025).
19. **1st** From Atomic Motif to Realistic Single Atom Catalysts through Machine Learning Interatomic Potentials. **ACS Energy Letters**, 10, 6288-6296. (IF = 18.9). **Choung, S.<sup>†</sup>**, Kim, M. <sup>†</sup>, Moon, J. <sup>†</sup>, Han, J. W.\* (2025).
18. CatBench: Benchmark framework of Machine Learning Interatomic Potentials for Adsorption Energy Predictions in Heterogeneous Catalysis. **Cell Reports Physical Science**, 6, 102968. [[Code](#)] (IF = 7.3). Moon, J., Jeon, U., **Choung, S.**, Han, J. W.\* (2025).
17. **1st** Partially reduced PdOx nanoparticles strongly interacting with defect-rich ceria via dynamic redox pulse for complete methane oxidation. **Applied Catalysis B: Environmental**, 379, 125672. [[Code](#)] (IF = 21.1). Ryu, S.<sup>†</sup>, **Choung, S.<sup>†</sup>**, Choi, Y., Lee, H., Choi, J., Han, J. W.\* , Jeong, H.\* (2025).
16. **1st** Engineering Active-Sites into Iron Hydroxide/Pt-based Nanocatalysts to Enrich the Oxygen Reduction Reaction. **ACS Applied Materials & Interfaces**, 17, 40517-40526. (IF = 8.2). Maiti, S.<sup>†</sup>, **Choung, S.<sup>†</sup>**, Maiti, K., Curnan, M. T., Hur, J., Han, J. W.\* (2025).
15. Quantity effect of heteroatom incorporation on the oxygen evolution mechanism in ruthenium oxide. **Chem**, 11, 102367. (IF = 19.6). Jun, H.<sup>†</sup>, Kang, E.<sup>†</sup>, Moon, J.<sup>†</sup>, Kim, H., Han, S., **Choung, S.**, Kim, S., Yi, S. Y., Kang, E., Choi, C. H.\* (2025).
14. **1st** Highly Durable Rh Single Atom Catalyst Modulated by Surface Defects on Fe-Ce Oxide Solid Solution. **Angew. Chem. Int. Ed.**, 64, e202421218. (IF = 17.0). Kim, G.<sup>†</sup>, **Choung, S.<sup>†</sup>**, Hwang, J., Choi, Y., Kim, S., Shin, D., Han, J. W.\* , Lee, H.\* (2025).
13. Surface Defect Recovery in Perovskite Nanocrystals with Excess Halide for Core-Shell Structure. **ACS Energy Letters**, 9, 5413-5420. (IF = 18.9). Lee, D. H., Jeong, W. H., **Choung, S.**, Jang, J. W., Lee, G., Song, H., Han, S., Seok, G. E., Kim, J., Han, M.\* (2024).
12. **1st** Rise of machine learning potentials in heterogeneous catalysis: Developments, applications, and prospects. **Chemical Engineering Journal**, 494, 152797. (IF = 13.2). **Choung, S.**, Park, W., Moon, J., Han, J. W.\* (2024).
11. **1st** Theoretical tuning of local coordination environment of metal-nitrogen doped carbon catalysts for selective chlorine-evolution reaction. **Catalysis Today**, 425, 114358. [[Code](#)] (IF = 5.3). **Choung, S.**, Yang, H., Moon, J., Park, W., June, H., Lim, C., Han, J. W.\* (2024).
10. Atomically Dispersed Ru-doped Ti<sub>4</sub>O<sub>7</sub> Electrocatalysts for Chlorine Evolution Reaction with a Universal Activity. **Small**, 20, 2401248. (IF = 12.1). Lee, W., **Choung, S.**, Kim, S., Han, J. W., Cho, K.\* (2024).
9. Accelerating Li-based battery design by computationally engineering materials. **Chem**, 9, 3415-3460. (IF = 19.6). Maiti, S., Curnan, M. T., Maiti, K., **Choung, S.**, Han, J. W.\* (2023).
8. Structural effects of nitrogen-doped titanium oxide supports on stabilization of ruthenium active species in carbon dioxide hydrogenation to formate. **Applied Catalysis B: Environmental**, 335, 122873. (IF = 21.1). Park, K., Lee, K. R., Ahn, S., Kim, S., Haider, A., **Choung, S.**, Han, J. W., Jung, K.\* (2023).
7. **1st** Synthesis of metal cation doped nanoparticles for single atom alloy catalysts using spontaneous cation exchange. **Journal of Materials Chemistry A**, 11, 2857-2867. (IF = 9.5). Xiao, X. <sup>†</sup>, Kang, S. <sup>†</sup>, **Choung, S.<sup>†</sup>**, Han, J. W.\* , Park, J.\* , Yu, T.\* (2023).
6. **1st** Unveiling the catalyst deactivation mechanism in the non-oxidative dehydrogenation of light alkanes on Rh (111): Density functional theory and kinetic Monte Carlo study. **Catalysis Today**, 411, 113819. (IF = 5.3). **Choung, S.**, Kim, Y., Moon, J., Roh, J., Hwang, J., Han, J. W.\* (2023).
5. Role of an Interface for Hydrogen Production Reaction over Size-Controlled Supported Metal Catalysts. **ACS Catalysis**, 12(13), 8082-8093. (IF = 13.1). Shin, D., Huang, R., Jang, M. G., **Choung, S.**, Kim, Y., Sung, K., Kim, T. Y., Han, J. W.\* (2022).
4. Structural effect of Nitrogen/Carbon on the stability of anchored Ru catalysts for CO<sub>2</sub> hydrogenation to formate. **Chemical Engineering Journal**, 433, 133571. (IF = 13.2). Jaleel, A., Haider, A., Van Nguyen, C., Lee, K. R., **Choung, S.**, Han, J. W., Baek, S., Shin, C., Jung, K.\* (2022).
3. Continuous Oxygen Vacancy Gradient in TiO<sub>2</sub> Photoelectrodes by a Photoelectrochemical-Driven "Self-Purification" Process. **Advanced Energy Materials**, 12(7), 2103495. (IF = 26.0). Kim, K. H., Choi, C., **Choung, S.**, Cho, Y., Kim, S., Oh, C., Lee, K., Lee, C., Zhang, K., Han, J. W.\* (2022).
2. Tuning electrochemical water oxidation towards ozone evolution with heterojunction anode architectures.

**Journal of Materials Chemistry A**, 10(33), 17132-17141. (IF = 9.5). Kim, S., **Choung, S.**, Lee, W., Bae, S., Han, J. W.\*, Cho, K.\* (2022).

1. **1st** Design principles of noble metal-free electrocatalysts for hydrogen production in alkaline media: combining theory and experiment. **Nanoscale Advances**, 3(24), 6797-6826. (IF = 4.7). Jung, H. †, **Choung, S.†**, Han, J. W.\* (2021).

## Conference Presentations (14 oral)

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21. **Choung, S.** (2026). Compressing Machine Learning Interatomic Potentials via Relational Knowledge Distillation for High-Throughput Electrocatalyst Screening (Oral). ACS Fall, Chicago.
20. **Choung, S.** (2026). Angular Relational Knowledge Distillation for Accelerating Equivariant Graph Neural Network Potentials (Oral). KSIEC Spring Meeting.
19. **Choung, S.** (2026). Distilling Machine Learning Interatomic Potentials for Scalable Catalyst Discovery (Oral). KIM Spring Meeting.
18. **Choung, S.** (2025). Ceria Nanoarchitectures with Enhanced Oxygen Mobility for Redox Reactions (Oral). APCAT-10 & ISSAC-4, Singapore.
17. **Choung, S.** (2025). Atomistic Intelligence for Sustainable Chemical Engineering: Ontology-Guided Discovery and Multiscale Modeling in Catalysis (Oral). AIChE, Boston.
16. **Choung, S.** (2025). Graph Neural Network Distillation for Scalable Catalytic Material Exploration (Oral). AIChE, Boston.
15. **Choung, S.** (2025). Graph Neural Networks for Exploring Active Sites in Single-Atom and Exsolution Catalysts (Oral). AIChE, Boston.
14. **Choung, S.** (2025). Highly Reactive Ceria Nanomaces for Enhanced Lattice Oxygen Kinetics (Oral). NAM29, Atlanta.
13. **Choung, S.** (2025). Fast and Domain-Accurate Graph Neural Network for Pt Single Atom Systems via Transfer Learning (Poster). NAM29, Atlanta.
12. **Choung, S.** (2025). Decoding Ni Exsolution in Ceria Catalysts Using a Kinetics-Aware Graph Neural Network (Poster). KSIEC, Jeju.
11. **Choung, S.** (2025). Kinetics-based Graph Neural Network Simulation of Nickel Exsolution Growth in Ceria Catalysts (Oral). KICHe, Daegu.
10. **Choung, S.** (2024). Machine Learning Potentials in Multiscale Simulation of Heterogeneous Catalysis (Oral). AIChE, San Diego.
9. **Choung, S.** (2024). Lattice Oxygen Kinetics in Nanostructured Ceria: GNN Multi-scale Simulations and In-situ DRIFT (Oral). AIChE, San Diego.
8. **Choung, S.** (2024). Unravelling the Lattice Oxygen Activation in Nanostructured Ceria using GNN Multi-scale Simulations (Oral). KICHe, Busan.
7. **Choung, S.** (2023). Breaking Scaling Relation of Electrochemical ORR Catalysis through Iron-Hydroxide Decoration (Oral). NANO KOREA, Seoul.
6. **Choung, S.** (2023). Mechanistic Origin of Selective Electrochemical Ozone Evolution over Ni-Sb-SnO<sub>2</sub> (Oral). NAM28, Providence.
5. **Choung, S.** (2022). First-Principles Design of Rh-based Alloy Catalysts for Selective Propane Dehydrogenation (Oral). AIChE, Phoenix.
4. **Choung, S.** (2022). First-principles Design of Rh-based Alloy Catalysts for Selective Propane Dehydrogenation (Oral). KICHe, Jeju.
3. **Choung, S.** (2021). DFT Study of the Pronounced Effect of Sn on RhSn Catalysts for Propane Dehydrogenation (Oral). IUMRS-ICA, Jeju.
2. **Choung, S.** (2021). DFT Study of Selective Electrochemical Ozone Production on SiOx deposited Ni-Sb-SnO<sub>2</sub> (Poster). KICHe, Busan.
1. **Choung, S.** (2021). Revealing Highly Active Origin of Rhodium for Catalytic Dehydrogenation Using Kinetic Monte Carlo (Poster). KICHe, Gwangju.

## Skills

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- **Domain Expertise:** Chemical Reaction Mechanisms, Catalyst/Material Screening, Heterogeneous Catalysis, Electrocatalysis, Surface Chemistry, High-throughput Screening
- **Experimental Literacy:** 17 publications from experiment-theory collaboration. Catalyst reaction networks, synthesis, material reconstruction, phase transitions, structural heterogeneity. Characterization literacy: X-ray (XPS, XAS, XRD), TEM, Raman, IR, catalytic reaction testing, electrochemical measurements
- **Computational Tools:** Python (ASE, E3nn, FairChem, MACE, Pymatgen/Materials Project), DFT (VASP, GPAW, Gaussian), MD (LAMMPS), Reaction Pathway (NEB), Kinetic Monte Carlo, Free Energy/Metadynamics

- **MLIP Capacity:** Fluent in equivariant GNN models (EquiformerV2, eSEN-based). Domain-targeted inference, fine-tuning, distillation, transfer learning, knowledge extraction from latent embeddings. PyTorch, PyTorch Geometric, Scikit-learn
- **Language Model Orchestration:** LLM orchestration (LangChain, LangGraph) with Gemini/GPT/Claude. Fluent in MCP/Skills
- **Infrastructure:** High-throughput DFT/MD on HPC. Multi-node H100 parallel training on KISTI national supercomputer. Local multi-GPU clusters (A6000/L40S). Workflow automation for large-scale screening campaigns

## Awards & Honors

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- **Poster Presentation Excellence Award** 2025  
KSIEC
- **Oral Presentation Award** Fall 2021  
IUMRS-ICA
- **Poster Presentation Excellence Award** Fall 2021  
KICHe Fall Meeting
- **Poster Presentation Excellence Award** Spring 2021  
KICHe Spring Meeting
- **POSCO Creative Research Program 3rd Prize** Feb. 2019  
POSCO
- **GS Caltex Project Excellence Award** Dec. 2018  
GS Caltex-SNU Program

## Teaching

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- **Seoul National University** Fall 2024  
TA - Computational Materials and Data Science ([🔗 Course Materials](#)) Seoul, South Korea
- **POSTECH** Fall 2023  
TA - Physical Chemistry Experiment Pohang, South Korea
- **POSTECH** Fall 2021  
TA - Molecular Simulation Pohang, South Korea