

Seokhyun Choung

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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 (25 PUBLISHED, 2 IN REVISION, 1 SUBMITTED)

† Equal contribution, * Corresponding author

[Sub.] Kim, H.[†], **Choung, S.[†]**, Ma, R.[†], Fu, Z., Han, J. W.^{*}, An, J.^{*}, Bu, Y.^{*} (2026). [Phase-transformation-enabled linear junctions drive high-rate electrosynthesis of H₂O₂](#). Submitted.

[Rev.] Kim, J.[†], Kim, Y.[†], Oh D., **Choung, S.**, Lee H., Lee H., Lee E., Kim J., Yoon S.^{*}, Han J. W.^{*}, An K.^{*} (2026). [TiO₂-facet-dependent reconstruction of Pt nanoparticles during CO oxidation](#). *Nature Communications*, in revision.

[Rev.] Kim, G.[†], Shin, H.[†], **Choung, S.[†]**, D'Andria, M., Han, J. W.^{*}, Güntner, A. T.^{*} (2026). [High-performance gas sensors through predictive material design](#). *Nature Sensors*, in revision.

- [25] **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). Hierarchical ceria nanoarchitecture enabling accelerated lattice oxygen dynamics for advanced redox reactions. *Nature Communications*, accepted. [ **Code**] (IF = 15.7)
- [24] Lim, H.[†], **Choung, S.[†]**, Moon, J., Han, J. W.* (2026). Angular relational knowledge distillation of machine learning interatomic potentials for scalable catalyst exploration. *npj Computational Materials*, accepted. [ **Code**] (IF = 11.9)
- [23] **Choung, S.[†]**, Kim, S.[†], Lee, J., Cho, K.* , Han, J. W.* (2026). Dynamic Hydroxyl Bridge Mechanism for Selective Ozone Evolution on Ni-Sb-SnO₂. *Applied Catalysis B: Environment and Energy*, 391, 126646. (IF = 21.1)
- [22] **Choung, S.**, Kim, H., Kim, J., Han, J. W.* (2026). CatAgent: Multi-Agent Orchestration for Electrocatalyst Discovery. *Workshop on AI for Accelerated Materials Design, ICLR 2026*.
- [21] Choi, Y.[†], **Choung, S.[†]**, Han, J.[†], Hwang, J., Jin, H., Kim, Y., Kim, J., Park, J. Y.* , Han, J. W.* , Lee, H.* (2026). Understanding oxygen transfer on ceria with Pt single atoms for surface reaction. *Nature Communications*, 17, 298. [ **Code**] (IF = 15.7)
- [20] Lim, H., **Choung, S.**, Han, J. W.* (2025). FORK: First-Order Relational Knowledge Distillation for Machine Learning Interatomic Potentials. *Workshop on AI for Accelerated Materials Design, NeurIPS 2025*. [ **Code**]
- [19] **Choung, S.[†]**, Kim, M. [†], Moon, J. [†], Han, J. W.* (2025). From Atomic Motif to Realistic Single Atom Catalysts through Machine Learning Interatomic Potentials. *ACS Energy Letters*, 10, 6288-6296. (IF = 18.9)
- [18] Moon, J., Jeon, U., **Choung, S.**, Han, J. W.* (2025). 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)
- [17] Ryu, S.[†], **Choung, S.[†]**, Choi, Y., Lee, H., Choi, J., Han, J. W.* , Jeong, H.* (2025). 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)
- [16] Maiti, S.[†], **Choung, S.[†]**, Maiti, K., Curnan, M. T., Hur, J., Han, J. W.* (2025). 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)
- [15] Jun, H.[†], Kang, E.[†], Moon, J.[†], Kim, H., Han, S., **Choung, S.**, Kim, S., Yi, S. Y., Kang, E., Choi, C. H.* (2025). Quantity effect of heteroatom incorporation on the oxygen evolution mechanism in ruthenium oxide. *Chem*, 11, 102367. (IF = 19.6)
- [14] Kim, G., **Choung, S.**, Hwang, J., Choi, Y., Kim, S., Shin, D., Han, J. W.* , Lee, H.* (2025). 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)
- [13] 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). Surface Defect Recovery in Perovskite Nanocrystals with Excess Halide for Core-Shell Structure. *ACS Energy Letters*, 9, 5413-5420. (IF = 18.9)
- [12] **Choung, S.**, Park, W., Moon, J., Han, J. W.* (2024). Rise of machine learning potentials in heterogeneous catalysis: Developments, applications, and prospects. *Chemical Engineering Journal*, 494, 152797. (IF = 13.2)
- [11] **Choung, S.**, Yang, H., Moon, J., Park, W., June, H., Lim, C., Han, J. W.* (2024). 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)
- [10] Lee, W., **Choung, S.**, Kim, S., Han, J. W., Cho, K.* (2024). Atomically Dispersed Ru-doped Ti₄O₇ Electrocatalysts for Chlorine Evolution Reaction with a Universal Activity. *Small*, 20, 2401248. (IF = 12.1)
- [9] Maiti, S., Curnan, M. T., Maiti, K., **Choung, S.**, Han, J. W.* (2023). Accelerating Li-based battery design by computationally engineering materials. *Chem*, 9, 3415-3460. (IF = 19.6)
- [8] Park, K., Lee, K. R., Ahn, S., Kim, S., Haider, A., **Choung, S.**, Han, J. W., Jung, K.* (2023). 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)
- [7] Xiao, X. [†], Kang, S. [†], **Choung, S.[†]**, Han, J. W.* , Park, J.* , Yu, T.* (2023). 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)

- [6] **Choung, S.**, Kim, Y., Moon, J., Roh, J., Hwang, J., Han, J. W.* (2023). 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)
- [5] Shin, D., Huang, R., Jang, M. G., **Choung, S.**, Kim, Y., Sung, K., Kim, T. Y., Han, J. W.* (2022). Role of an Interface for Hydrogen Production Reaction over Size-Controlled Supported Metal Catalysts. *ACS Catalysis*, 12(13), 8082-8093. (IF = 13.1)
- [4] Jaleel, A., Haider, A., Van Nguyen, C., Lee, K. R., **Choung, S.**, Han, J. W., Baek, S., Shin, C., Jung, K.* (2022). Structural effect of Nitrogen/Carbon on the stability of anchored Ru catalysts for CO₂ hydrogenation to formate. *Chemical Engineering Journal*, 433, 133571. (IF = 13.2)
- [3] Kim, K. H., Choi, C., **Choung, S.**, Cho, Y., Kim, S., Oh, C., Lee, K., Lee, C., Zhang, K., Han, J. W.* (2022). Continuous Oxygen Vacancy Gradient in TiO₂ Photoelectrodes by a Photoelectrochemical-Driven "Self-Purification" Process. *Advanced Energy Materials*, 12(7), 2103495. (IF = 26.0)
- [2] Kim, S., **Choung, S.**, Lee, W., Bae, S., Han, J. W.*, Cho, K.* (2022). Tuning electrochemical water oxidation towards ozone evolution with heterojunction anode architectures. *Journal of Materials Chemistry A*, 10(33), 17132-17141. (IF = 9.5)
- [1] Jung, H. [†], **Choung, S.**[†], Han, J. W.* (2021). 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)

CONFERENCE PRESENTATIONS

- [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 (Invited). 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 (Invited). 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-SnO₂ (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 SiO_x deposited Ni-Sb-SnO₂](#) (Poster). *KIChE*, Busan.
- [1] **Choung, S.** (2021). [Revealing Highly Active Origin of Rhodium for Catalytic Dehydrogenation Using Kinetic Monte Carlo](#) (Poster). *KIChE*, Gwangju.

SKILLS

- **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
<i>KSIEC</i> | 2025 |
| • Oral Presentation Award
<i>IUMRS-ICA</i> | Fall 2021 |
| • Poster Presentation Excellence Award
<i>KIChE Fall Meeting</i> | Fall 2021 |
| • Poster Presentation Excellence Award
<i>KIChE Spring Meeting</i> | Spring 2021 |
| • POSCO Creative Research Program 3rd Prize
<i>POSCO</i> | Feb. 2019 |
| • GS Caltex Project Excellence Award
<i>GS Caltex-SNU Program</i> | Dec. 2018 |

TEACHING

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|---|----------------------------------|
| • Seoul National University
<i>TA - Computational Materials and Data Science ( Course Materials)</i> | Fall 2024
Seoul, South Korea |
| • POSTECH
<i>TA - Physical Chemistry Experiment</i> | Fall 2023
Pohang, South Korea |
| • POSTECH
<i>TA - Molecular Simulation</i> | Fall 2021
Pohang, South Korea |