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. I leverage **machine learning** (Distillation/Fine-tuning/Generative diffusion/-Multiscale simulation) and ***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 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 (24 published, 3 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 H_2O_2. *Nature Nanotechnology*, submitted.

[Rev.] **Choung, S.†**, Jang, M. G.†, Kim, Y.†, 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*, in revision. [**Code**]

[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). TiO_2-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*, under review.

[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**]

[23] **Choung, S.**†, Kim, S.†, Lee, J., Cho, K.*, Han, J. W.* (2026). Dynamic Hydroxyl Bridge Mechanism for Selective Ozone Evolution on Ni-Sb-SnO_2. *Applied Catalysis B: Environment and Energy*, 391, 126646.

[22] **Choung, S.**, Kim, H., Kim, J., Han, J. W.* (2026). CatAgent: Multi-Agent Orchestration for Electrocatalyst Discovery. *ICLR 2026 Workshop AI4Mat*.

[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**]

[20] Lim, H., **Choung, S.**, Han, J. W.*(2025). FORK: First-Order Relational Knowledge Distillation for Machine Learning Interatomic Potentials. *AI4Mat-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.

[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**]

[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**]

[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.

[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.

[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.

[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.

[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.

[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**]

[10] Lee, W., **Choung, S.**, Kim, S., Han, J. W., Cho, K.* (2024). Atomically Dispersed Ru-doped Ti_4O_7 Electrocatalysts for Chlorine Evolution Reaction with a Universal Activity. *Small*, 20, 2401248.

[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.

[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.

[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.

[6] **Choung, S.**, Kim, Y., Moon, J., Roh, J., Hwang, J., Han, J. W.*(2023). Unveiling the catalyst deac-

tivation mechanism in the non-oxidative dehydrogenation of light alkanes on Rh (111): Density functional theory and kinetic Monte Carlo study. *Catalysis Today*, 411, 113819.

[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.

[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 CO_2 hydrogenation to formate. *Chemical Engineering Journal*, 433, 133571.

[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 TiO_2 Photoelectrodes by a Photoelectrochemical-Driven "Self-Purification" Process. *Advanced Energy Materials*, 12(7), 2103495.

[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.

[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.

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-SnO_2 (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_2 (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

- **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

- **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