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 (16 first-author, 1 in revision, 2 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).

In review. 1st Phase-transformation-enabled linear junctions drive high-rate electrosynthesis of H_2O_2. **Nature Communications**, in revision. Kim, H.†, **Choung, S.**†, Ma, R.†, Fu, Z., Han, J. W.*, An, J.*, Bu, Y.* (2026).

29. HEAgent: Autonomous Large Language Model-Driven Framework for High-Entropy Alloy Electrocatalyst Discovery. **Workshop on AI for Accelerated Materials Design, NeurIPS 2026**, accepted. Kim, H., **Choung, S.**, Han, J. W.* (2026).
28. 1st ASE-Bench: An Atomic Simulation Benchmark for Agentic Materials Discovery. **Workshop on AI for Accelerated Materials Design, NeurIPS 2026**, accepted. **Choung, S.** (2026).
27. TiO_2-facet-dependent reconstruction of Pt nanoparticles during CO oxidation. **Nature Communications**. (IF = 15.7). 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**. 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 activation for efficient redox reactions. **Nature Communications**, 17, 5868. [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**, 12, 193. [Code] (IF = 11.9). Lim, H.†, **Choung, S.**†, Moon, J., Han, J. W.* (2026).
23. **1st** Dynamic Hydroxyl Bridge Mechanism for Selective Ozone Evolution on Ni-Sb-SnO_2. **Applied Catalysis B: Environment and Energy**, 391, 126646. (IF = 21.1). **Choung, S.**†, Kim, S.†, 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.†, **Choung, S.**†, Han, J.†, 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.**†, Kim, M. †, Moon, J. †, 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.†, **Choung, S.**†, 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.†, **Choung, S.**†, 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.†, Kang, E.†, Moon, J.†, 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.†, **Choung, S.**†, 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_4O_7 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. †, Kang, S. †, **Choung, S.**†, 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_2 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_2 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).

Conferences and Invited Talks (18 oral, 6 posters, 5 invited)

Inv. **Choung, S.** (2026). Angular Relational Knowledge Distillation of Machine Learning Interatomic Potentials for Scalable Catalyst Exploration (Invited Talk). LeMaterial Reading Group, Entalpic & The AI Alliance, Online.

Inv. **Choung, S.** (2026). How Does CCEL Advance Catalysis and Battery Technology using Matlantis? (Invited Industry Seminar). Matlantis-CCEL SNU Technical Meeting, Preferred Networks.

Inv. **Choung, S.** (2025). How Does CCEL Advance Catalysis and Battery Technology using Matlantis? (Invited Industry Seminar). Matlantis-CCEL SNU Technical Meeting, Preferred Networks.

Inv. **Choung, S.** (2025). Machine Learning Potentials for Material Discovery (Invited Seminar). 2D Materials Workshop, South Korea.

Inv. **Choung, S.** (2024). Machine Learning Interatomic Potentials for Accelerated Catalyst and Materials Discovery (Invited Industry Seminar). CCEL-PFP Technical Meeting, Preferred Networks.

28. **Choung, S.** (2026). Atomistic Intelligence for Catalysis: Scalable, Generative, and Agentic Discovery (Poster). AIChE, Minneapolis.
27. **Choung, S.** (2026). Harnessing LLM Agents for Autonomous Catalytic Materials Discovery (Oral). KSIEC Fall Meeting, Busan.
26. **Choung, S.** (2026). Structural Engineering of Ceria via Machine Learning Interatomic Potentials (Oral). KSIEC Fall Meeting, Busan.
25. **Choung, S.** (2026). Atomistic Agents for Autonomous Catalyst Discovery (Oral). KIChE Fall Meeting, Busan.
24. **Choung, S.** (2026). Atomistic Agents for Autonomous Exploration of Solid Oxide Cell Materials (Oral). The Korean Ceramic Society Fall Meeting, Seoul.
23. **Choung, S.** (2026). Atomistic Agents for Autonomous Catalyst Discovery (Oral). AI4Sci Korea, Seoul.
22. **Choung, S.** (2026). Compressing Machine Learning Interatomic Potentials via Relational Knowledge Distillation for High-Throughput Electrocatalyst Screening (Poster). ACS Fall, Chicago.
21. **Choung, S.** (2026). Atomistic Intelligence for Structural Engineering of Ceramic Materials (Poster). The 3rd K-SOC Symposium, Cheongju, South Korea.
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_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