

# Seokhyun Choung

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

## PROFILE

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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

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- **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

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- **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

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- **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)

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† 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<sub>2</sub>O<sub>2</sub>. 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). TiO<sub>2</sub>-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.**<sup>†</sup>, Kim, Y.<sup>†</sup>, Jang, M. G.<sup>†</sup>, 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.<sup>†</sup>, **Choung, S.**<sup>†</sup>, 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.**<sup>†</sup>, Kim, S.<sup>†</sup>, Lee, J., Cho, K.\* , Han, J. W.\* (2026). 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)
- [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.<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). 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.**<sup>†</sup>, Kim, M. <sup>†</sup>, Moon, J. <sup>†</sup>, 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.<sup>†</sup>, **Choung, S.**<sup>†</sup>, 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.<sup>†</sup>, **Choung, S.**<sup>†</sup>, 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.<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). 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 Ti<sub>4</sub>O<sub>7</sub> 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. <sup>†</sup>, Kang, S. <sup>†</sup>, **Choung, S.**<sup>†</sup>, 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 CO<sub>2</sub> 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 TiO<sub>2</sub> 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

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- [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<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 SiO<sub>x</sub> 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