

Seokhyun Choung

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Research Institute of Advanced Material, Seoul National University

PROFILE

Post-Doctoral Researcher developing next-generation catalysts to combat climate change through computational design. I leverage machine learning ([Diffusion/Distillation/Transfer Learning](#)) and quantum mechanical calculations to discover efficient catalytic materials for clean fuel production and sustainable chemical processes.

EXPERIENCE

- Seoul National University** 2024 – Present
Post-Doctoral Researcher Seoul, South Korea
 - Multiscale catalysis simulation for catalyst and energy materials design
 - Development of machine learned interatomic potentials for heterogeneous catalysis (Distillation, Diffusion, Transfer Learning, Catalyst Benchmark)

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
 - Mechanism study of Platinum Catalyst in Oxygen Reduction Reaction using DFT approach
 - Exchange semester at Seoul National University (2018 Fall) and Technical University of Denmark (2019 Fall)

TEACHING EXPERIENCE

- Seoul National University** Fall 2024
Teaching Assistant - Computational Materials and Data Science Seoul, South Korea
- POSTECH** Fall 2023
Teaching Assistant - Physical Chemistry Experiment Pohang, South Korea
- POSTECH** Fall 2021
Teaching Assistant - Molecular Simulation Pohang, South Korea

PUBLICATIONS (19 PUBLISHED, 3 IN REVISION, 1 SUBMITTED)

[†] Equal contribution, * Corresponding author

- [Submitted] Kim, H.[†], **Choung, S.[†]**, Ma, R., Fu, Z., Han, J. W.* , An, J.* , Bu, Y.* (2025). [Phase-transformation-enabled linear junctions drive high-rate electrosynthesis of H₂O₂](#).
- [revision] **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*, in revision.
- [revision] Kim, J.[†], Kim, Y.[†], Oh D., **Choung, S.**, Lee H., Lee H., Lee E., Kim J., Yoon S.* , Han J. W.* , An K.* (2025). [TiO₂-facet-dependent reconstruction of Pt nanoparticles during CO oxidation](#). *Nature Communications*, in revision.
- [revision] **Choung, S.[†]**, Jang, M. G.[†], Kim, Y., Lee, T., Park, W., Kim, M., Seo, O., Watanabe, T., Kumara, L. S. R., Matsumura, D., Kim, T. Y., Han, J. W.* (2025). [Hierarchical ceria nanoarchitecture enabling accelerated lattice oxygen dynamics for advanced redox reactions](#). *Nature Catalysis*, in revision.
- [1] Choi, Y.[†], **Choung, S.[†]**, Han, J.[†], Hwang, J., Kim, S., Park, J. Y* , Han, J. W.* , Lee, H.* (2025). [Understanding oxygen transfer on ceria with Pt single atoms for surface reaction](#). *Nature Communications*, in press.
- [2] 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*, in press.
- [3] 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.
- [4] 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 Material Interfaces*, 17, 40517-40526.

- [5] 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.
- [6] 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.
- [7] 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.
- [8] **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.
- [9] **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.
- [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.
- [11] 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.
- [12] 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.
- [13] 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.
- [14] **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.
- [15] 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.
- [16] 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.
- [17] 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.
- [18] 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.
- [19] 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

- [1] **Choung, S.** (2025). [Graph Neural Network Distillation for Scalable Catalytic Material Exploration](#) (Oral Presentation). *American Institute of Chemical Engineers (AIChE)*, Boston, United States.
- [2] **Choung, S.** (2025). [Graph Neural Networks for Exploring Active Sites in Single-Atom and Exsolution Catalysts for Redox Reactions](#) (Oral Presentation). *American Institute of Chemical Engineers (AIChE)*, Boston, United States.
- [3] **Choung, S.** (2025). [Fast and Domain-Accurate Graph Neural Network for Pt Single Atom Systems via Transfer Learning](#) (Poster). *The 29th North American Catalysis Society Meeting (NAM29)*, Atlanta, United States.
- [4] **Choung, S.** (2025). [Decoding Ni Exsolution in Ceria Catalysts Using a Kinetics-Aware Graph Neural Network](#) (Poster). *2025 The Korean Society of Industrial and Engineering Chemistry (KSIEC)*, Jeju, South Korea.
- [5] **Choung, S.** (2025). [Kinetics-based Graph Neural Network Simulation of Nickel Exsolution Growth in Ceria Catalysts](#) (Oral Presentation). *Korean Institute of Chemical Engineers (KICHE)*, Daegu, South Korea.
- [6] **Choung, S.** (2025). [Machine Learning Potentials in Multiscale Simulation of Heterogeneous Catalysis using Machine Learning Potential](#) (Meet the Faculty Session). *American Institute of Chemical Engineers (AIChE)*, San Diego, United States.

- [7] **Choung, S.** (2024). [Unravelling the Lattice Oxygen Activation in Nanostructured Ceria using Graph Neural Network Multi-scale Simulations](#) (Oral Presentation). *Korean Institute of Chemical Engineers (KICHE)*, Busan, South Korea.
- [8] **Choung, S.** (2024). [Lattice Oxygen Kinetics in Nanostructured Ceria: Combining Graph Neural Network Multi-scale Simulations and In-situ DRIFT Characterization](#) (Oral Presentation). *American Institute of Chemical Engineers (AIChE)*, San Diego, United States.
- [9] **Choung, S.** (2024). [Lattice Oxygen Kinetics in Nanostructured Ceria: Combining Graph Neural Network Multi-scale Simulations and In-situ DRIFT Characterization](#) (Oral Presentation). *American Institute of Chemical Engineers (AIChE)*, San Diego, United States.
- [10] **Choung, S.** (2023). [Breaking Scaling Relation of Electrochemical Oxygen Reduction Catalysis through Iron-Hydroxide Decoration](#) (Oral Presentation). *NANO KOREA 2023 Symposium*, Seoul, South Korea.
- [11] **Choung, S.** (2023). [Mechanistic Origin of Selective and Active Electrochemical Ozone Evolution Reaction over Ni-Sb-SnO₂ Electrode](#) (Oral Presentation). *The 28th North American Catalysis Society Meeting (NAM28)*, Providence, Rhode Island, United States.
- [12] **Choung, S.** (2022). [First-Principles Design of Rh-based Alloy Catalysts for Selective Propane Dehydrogenation](#) (Oral Presentation). *American Institute of Chemical Engineers (AIChE)*, Arizona, United States.
- [13] **Choung, S.** (2022). [First-principles Design of Rh-based Alloy Catalysts for Selective Propane Dehydrogenation](#) (Oral Presentation). *Korean Institute of Chemical Engineers (KICHE)*, Jeju, South Korea.
- [14] **Choung, S.** (2021). [Density Functional Theory Study of the Pronounced Effect of Sn on RhSn Catalysts for Propane Dehydrogenation](#) (Oral Presentation). *International Union of Materials Research Societies - International Conference in Asia (IUMRS-ICA)*, Jeju, South Korea.
- [15] **Choung, S.** (2021). [Density Functional Theory Study of selective electrochemical ozone production on SiOx deposited Ni-Sb-SnO₂](#) (Poster). *Korean Institute of Chemical Engineers (KICHE)*, Busan, South Korea.
- [16] **Choung, S.** (2021). [Revealing Highly Active Origin of Rhodium for Catalytic Dehydrogenation of Light Alkanes Using Kinetic Monte Carlo Simulation](#) (Poster). *Korean Institute of Chemical Engineers (KICHE)*, Gwangju, South Korea.

SKILLS

- **Computational Methods:** Density Functional Theory (VASP, GPAW, ASE), Machine Learning Potentials, Molecular Dynamics, Kinetic Monte Carlo, Kinetic Modeling, High-throughput Screening
- **Machine Learning/AI:** PyTorch, Scikit-learn, Deep Learning, Transfer Learning, Knowledge Distillation, Graph Neural Networks (GemNet-OC, EquiformerV2)
- **Programming Languages:** Python (Advanced), C++ (Intermediate), MATLAB, Bash scripting
- **Research Expertise:** Heterogeneous Catalysis, Electrocatalysis (ORR, OER, HER, CER), Thermocatalysis (DRM, WGS, CO oxidation), Single-Atom Catalysts, Exsolution Catalysts, Surface Science, Materials Informatics
- **Languages:** Korean (Native), English (Fluent)