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, multiscale simulations, and ab-initio 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 learning potentials for heterogeneous catalysis

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 (17 published, 1 in revision, 3 submitted)

[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 H_2O_2.

[Submitted] **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.

[Submitted] 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.

[Revision] 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 Rep. Phys. Sci.*.

[1] 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. *Appl. Catal. B-Environ. Energy*, 379, 125672.

[2] 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 Appl. Mater. Interfaces*, 17, 40517-40526.

[3] Jun, H.†, Kang, E.†, Moon, J.†, Kim, H., Han, S., **Choung, S.**, Kim, S., Yi, S. Y., Kang, E., Choi, C. H.*, Han, J. W.*, Lee, J.* (2025). Quantity effect of heteroatom incorporation on the oxygen evolution mechanism in ruthenium oxide. *Chem*, 11, 102367.

[4] 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, 2401248.

[5] Lee, D. H., Jeong, W. H., **Choung, S.**, Jang, J. W., Lee, G., Song, H., Han, S., Seok, G. E., Kim, J., Han, M., et al. (2024). Surface Defect Recovery in Perovskite Nanocrystals with Excess Halide for Core–Shell Structure. *ACS Energy Letters*, 9, 5413-5420.

[6] **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.

[7] **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.

[8] 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.

[10] 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.

[11] 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.

[12] **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.

[13] 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.

[14] 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.

[15] 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.

[16] 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.

[17] 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). Highly Reactive Ceria Nanomaces for Enhanced Lattice Oxygen Kinetics for Oxidation Reactions (Oral Presentation). *The 29th North American Catalysis Society Meeting (NAM29)*, Atlanta, United States.

[2] **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.

[3] **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.

[4] **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.

[5] **Choung, S.** (2024). 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.

[6] **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.

[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.** (2023). Breaking Scaling Relation of Electrochemical Oxygen Reduction Catalysis through Iron-Hydroxide Decoration (Oral Presentation). *NANO KOREA 2023 Symposium*, Seoul, South Korea.

[9] **Choung, S.** (2023). Mechanistic Origin of Selective and Active Electrochemical Ozone Evolution Reaction over Ni-Sb-SnO_2 Electrode (Oral Presentation). *The 28th North American Catalysis Society Meeting (NAM28)*, Providence, Rhode Island, United States.

[10] **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.

[11] **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.

[12] **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.

[13] **Choung, S.** (2021). Density Functional Theory Study of selective electrochemical ozone production on SiOx deposited Ni-Sb-SnO_2 (Poster). *Korean Institute of Chemical Engineers (KICHE)*, Busan, South Korea.

[14] **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, WGSR, CO oxidation), Single-Atom Catalysts, Exsolution Catalysts, Surface Science, Materials Informatics
- **Languages:** Korean (Native), English (Fluent)