

Dongjae Shin

Postdoctoral Scholar, SUNCAT Center for Interface Science and Catalysis

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EDUCATION

- 2/2019 – 8/2023 **Ph.D.** in Chemical Engineering, **POSTECH**^a Pohang, Korea
 Advisor: [Jeong Woo Han](#)
 Thesis: AI-Aided Computational Design of Ceria-based High Performance Catalytic Materials
- 3/2016 – 2/2018 **M.S.** in Graduate School of EEWS, **KAIST**^b Daejeon, Korea
 Advisor: [Yong-Hoon Kim](#)
 Thesis: First-principles study of magnetism development in armchair graphene nanoribbons with edge functionalizations
- 3/2010 – 2/2016 **B.S.** in Chemical Engineering, **University of Seoul** Seoul, Korea
Cum Laude; top honor in Chemical Engineering

EXPERIENCE

- 2/2024 – **Postdoctoral Scholar**, Menlo Park, United States
 SUNCAT Center for Interface Science and Catalysis,
SLAC National Accelerator Laboratory, Stanford University
 Advisors: [Kirsten T. Winther](#) and [Christopher J. Tassone](#)
- 9/2023 – 1/2024 **Senior Researcher**, Seoul, Korea
 Department of Materials Science and Engineering, **SNU**^c
- 10/2018 – 2/2019 **Researcher**, Pohang, Korea
 Department of Chemical Engineering, **POSTECH**
- 3/2018 – 3/2018 **Contract Research Scientist**, Daejeon, Korea
 Applied Science Research Institute, **KAIST**
- 3/2012 – 12/2013 **Military Service**, Capital Defense Command, Republic of Korea Army Seoul, Korea
- 9/2011 – 12/2011 **Undergraduate Student Tutor**, School of General Education, **University of Seoul** (Subject: General Chemistry) Seoul, Korea

Note: 4/2018 – 9/2018 was dedicated to preparing for admission to POSTECH.

PUBLICATIONS (†: equal contribution, *: corresponding author)

22 papers including 11 first/co-first author papers, 2 submitted, 1 to be submitted

22. Tuning Cu-In Catalysts with Potassium: Enhancing Phase Separation and Bifunctionality for Low-Temperature Reverse Water-Gas Shift Reaction
 E. Erdem, J. Chen, **D. Shin**, D. U. Lee, R. Spurlock, S. -W. Lee, H. Badr, K. T. Winther, A. T. Rogala, and T. F. Jaramillo*, to be submitted (2025)
21. LABMATE: Language Model Based Multi-Agent System to Accelerate Catalysis Experiments
 A. Acharya, T. Vega, R. Ashraf, N. Isenberg, J. Strube, **D. Shin**, K. T. Winther, and R. Rallo*, submitted (2025)

^a POSTECH: Pohang University of Science and Technology

^b KAIST: Korea Advanced Institute of Science and Technology

^c SNU: Seoul National University

20. Quantifying Experimental Uncertainty in Catalyst Deactivation: Round-Robin Testing and Implications for Machine-Learned Prediction
S. Bac, **D. Shin**, S. Hong, A. Khan, Z. Chen, J. Heinlein, M. M. Albrechtsen, G. Barber, R. Rioux*, M. Cargnello*, C. J. Tassone*, S. R. Bare*, K. T. Winther*, P. Christopher*, A. S. Hoffman*, submitted (2025).
19. Highly Durable Rh Single Atom Catalyst Modulated by Surface Defects on Fe-Ce Oxide Solid Solution
G. Kim, S. Choung, J. Hwang, Y. Choi, S. Kim, **D. Shin**, J. W. Han*, H. Lee*, *Angew. Chem. Int. Ed.* 137 (2025) e202421218.
18. Unmatched Redox Activity of Palladium-Doped Indium Oxide Oxygen Carrier for Low-Temperature CO₂ Splitting
S. Park†, D. Oh†, M. G. Jang†, H. Seo, U. Kim, J. Ahn, Y. Choi, **D. Shin**, J. W. Han*, W. Jung*, and I.-D. Kim*, *ACS Nano* 18 (2024) 25577-25590.
Selected as a Supplementary cover
17. Atomically dispersed Rh catalysts formed on defective CeO₂ surfaces with hydroformylation activity
H. Lee†, **D. Shin**†, D. Oh†, B. Jeong, K. Y. Kim, C. Hur, J. W. Han*, and K. An*, *Chem. Eng. J.* 497 (2024) 153758.
16. Accelerated Structural Optimization for the Supported Metal System based on Hybrid Approach Combining Bayesian Optimization with Local Search
S. Bae†, **D. Shin**†, H. Kim, J. W. Han*, and J. M. Lee*, *J. Chem. Theory Comput.* 20 (2024) 2284-2296.
15. Surface Segregation Machine-Learned with Inexpensive Numerical Fingerprint for the Design of Alloy Catalysts
D. Shin, G. Choi, C. Hong, and J. W. Han*, *Mol. Catal.* 541 (2023) 113096.
14. Change in the Electronic Environment of the VO_x Active Center via Support Modification to Enhance Hg Oxidation Activity
W. Yeo†, **D. Shin**†, M. H. Kim, and J. W. Han*, *ACS Catal.* 13 (2023) 3775-3787.
Selected as a Supplementary cover
13. Modulating water gas shift reaction via strong interfacial interaction between defective oxide matrix and exsolved metal nanoparticles
H. Chen†, R. Huang†, M. G. Jang†, C. Lim, **D. Shin**, Q. Liu, H. Yang, Y. Chen*, and J. W. Han*, *J. Mater. Chem. A* 10 (2022) 24995-25008.
Selected as a Back cover
12. Role of an Interface for Hydrogen Production Reaction over Size-Controlled Supported Metal Catalysts
D. Shin†, R. Huang†, M. G. Jang, S. Choung, Y. Kim, K. Sung, T. Y. Kim, and J. W. Han*, *ACS Catal.* 12 (2022) 8082-8093.
11. Boosting Support Reducibility and Metal Dispersion by Exposed Surface Atom Control for Highly Active Supported Metal Catalysts
M. G. Jang†, S. Yoon†, **D. Shin**†, H. J. Kim, R. Huang, E. Yang, J. Kim, K.-S. Lee, K. An*, and J. W. Han*, *ACS Catal.* 12 (2022) 4402-4414.
10. Universally characterizing atomistic strain via simulation, statistics, and machine learning: low-angle grain boundaries
M. T. Curnan, **D. Shin**, W. A. Saidi, J. C. Yang, and J. W. Han*, *Acta Mater.* 226 (2022) 117635.
9. Alleviating Inhibitory Effect of H₂ on Low-Temperature Water-Gas Shift Reaction Activity of Pt/CeO₂ Catalyst by Forming CeO₂ Nano-Patches on Pt Nano-Particles
J. Lee, **D. Shin**, C. Li, E. W. Lee, J. M. Kim, J. W. Han, and D. H. Kim*, *Appl. Catal. B-Environ.* 305 (2022) 121038.
8. Facet-Dependent Mn Doping on Shaped Co₃O₄ Crystals for Catalytic Oxidation
J. Bae, **D. Shin**, H. Jeong, C. Choe, Y. Choi, J. W. Han, and H. Lee*, *ACS Catal.* 11 (2021).
Selected as a Supplementary cover
7. Structure-activity relationship of VO_x/TiO₂ catalysts for mercury oxidation: A DFT study
D. Shin, M. H. Kim, and J. W. Han*, *Appl. Surf. Sci.* 552 (2021) 149462.
6. Design of an Ultrastable and Highly Active Ceria Catalyst for CO Oxidation by Rare-Earth- and Transition-Metal Co-Doping

H. J. Kim†, **D. Shin**†, H. Jeong, M. G. Jang, H. Lee, and J. W. Han*, *ACS Catal.* 10 (2020) 14877-14886.

Selected as a Supplementary cover

5. Controlling the Oxidation State of Pt Single Atoms for Maximizing Catalytic Activity
H. Jeong†, **D. Shin**†, B. -S. Kim, J. Bae, S. Shin, C. Choe, J. W. Han*, and H. Lee*, *Angew. Chem. Int. Ed.* 59 (2020) 20691-20696.
4. Oxidative Methane Conversion to Ethane on Highly Oxidized Pd/CeO₂ Catalysts below 400 °C
G. Kwon†, **D. Shin**†, H. Jeong, S. K. Sahoo, J. Lee, G. Kim, J. Choi, D. H. Kim, J. W. Han*, and H. Lee*, *ChemSusChem* 13 (2020) 677-681.
3. Design of Ceria Catalysts for Low-Temperature CO Oxidation
H. J. Kim†, M. G. Jang†, **D. Shin**†, and J. W. Han*, *ChemCatChem* 12 (2020) 11-26.
Selected as a Front cover and Very Important Paper
2. Improved CO Oxidation via Surface Stabilization of Ceria Nanoparticles Induced by Rare-Earth Metal Dopants
K. -J. Noh†, K. Kim†, H. J. Kim†, **D. Shin**, and J. W. Han*, *ACS Appl. Nano Mater.* 2 (2019) 6473-6481.
1. Highly Water-Resistant La-doped Co₃O₄ catalyst for CO Oxidation
J. Bae, **D. Shin**, H. Jeong, B. -S. Kim, J. W. Han, and H. Lee*, *ACS Catal.* 9 (2019) 10093-10100.

INDEPENDENT FUNDING

1. **Principal Investigator**, *Active Learning-based Rational Design of Ceria Exsolution Catalysts*
- NRF Ph.D. Fellowship, National Research Foundation of Korea (NRF), 6/2022 – 5/2024, ~**32,000 USD**
- Developed an active learning framework to navigate metal exsolution condition for highly active catalysts

HONORS & AWARDS

1. **Graduate Research Award in Catalysis**, Korean Institute of Chemical Engineers (KIChE) Catalysis Division, 2/2023, Awarded to only three doctoral students annually
2. **Best Oral Award**, ENGE 2022, 11/2022
3. **NRF Ph.D. Fellowship**, National Research Foundation of Korea (NRF), 6/2022 – 5/2024, ~**32,000 USD**, ceased due to graduation
4. **Hoimyung Graduate Research Award**, KIChE, 4/2022
Awarded to only one graduate student semi-annually in catalysis division
5. **Best Publication Award for Graduate Student**, Department of Chem. Eng., POSTECH, 11/2021
6. **Best Publication Award for Graduate Student**, Department of Chem. Eng., POSTECH, 11/2020
7. **Best Poster Award**, The Korean Ceramic Society (KCerS) Conference, 11/2020
8. **Top Downloaded Paper 2018-2019**, ChemCatChem, Wiley, 4/2020
9. **Best Poster Award**, NANO KOREA 2017, 7/2017
10. **4th Place in Team Contest**, The 8th KIAS CAC Summer School on Parallel and Scientific Computing, 6/2017
11. **Government Scholarship**, Ministry of Education, Science and Technology, 2016 – 2018, ~**29,000 USD**
12. **Encouragement prize**, 5th EDISON Software Utilization Contest hosted by KISTI, 3/2016
13. **Scholarship for Excellent Achievement**, University of Seoul, 2014 – 2015, ~**1,800 USD**
14. **University Development Fund Scholarship**, University of Seoul, 2014, ~**1,200 USD**
15. **Seoul Mayor's Scholarship for Excellent Achievement**, University of Seoul, 2010 – 2011, ~**7,200 USD**
16. **Academic Excellence Award**, University of Seoul, 1st semester 2011, 2nd semester 2010, 1st semester 2010

PATENT

1. **KR 10-2021-0161145**, METHOD FOR STRUCTURE OPTIMIZATION IN ATOMIC LEVEL
J. M. Lee, S. Y. Bae, S. H. Lim, J. S. Shin, J. W. Han, **D. Shin**, 11/22/2021 (registered: **10-2684179**; 7/8/2024)

SELECTED PRESENTATION (INTERNATIONAL)

1. **SUNCAT Summer Institute 2025**, D. Shin, S. R. Bare, C. J. Tassone, and K. T. Winther, "Comparability Assessment of Catalyst Durability Tests from Multiple Laboratories to Generate High-Quality Data for Building Machine Learning Models", Menlo Park, CA, USA, 8/2025. (poster)
2. **29th North American Catalysis Society Meeting (NAM29)**, D. Shin, A. S. Hoffman, P. Christopher, M. Cargnello, S. R. Bare, C. J. Tassone, and K. T. Winther, "Generation of Catalysis Testing Data via Uncertainty Sampling to Build Machine Learning Models for Catalyst Durability", Atlanta, GA, USA, 6/2025. (oral)
3. **2024 MRS Fall Meeting**, D. Shin, C. J. Tassone, and K. T. Winther, "Uncertainty Sampling-Based Efficient Data Generation for Development of Machine Learning Model to Predict Catalyst Degradation", Boston, MA, USA, 12/2024. (oral)
4. **The International Conference on Electronic Materials and Nanotechnology for Green Environment (ENGE2022)**, D. Shin and J. W. Han, "Surface Segregation Prediction Machine-Learned with Inexpensive Numerical Fingerprint for Design of Alloy Catalysts", Jeju, Korea, 11/2022. (oral)
5. **Materials Challenges in Alternative and Renewable Energy (MCARE2022)**, D. Shin, R. Huang, M. G. Jang, S. Choung, Y. Kim, K. Sung, T. Y. Kim, and J. W. Han, "Role of Interface for the Water-Gas Shift Reaction over Size-Controlled Supported Metal Catalysts: A Combined Theoretical and Experimental Study", Busan, Korea, 8/2022. (oral)
6. **27th North American Catalysis Society Meeting (NAM27)**, D. Shin, R. Huang, M. G. Jang, S. Choung, Y. Kim, K. Sung, T. Y. Kim, and J. W. Han, "Role of Interface for the Water-Gas Shift Reaction over Size-Controlled Supported Metal Catalysts: A Combined Theoretical and Experimental Study", New York, NY, USA, 5/2022. (oral)
7. **POSTECH-SUNCAT Joint Workshop on Catalysis**, D. Shin, R. Huang, M. G. Jang, and J. W. Han, "Boosting Surface Properties of Supported Metal Catalysts for Water-Gas Shift Reaction: Combined Theoretical and Experimental Studies", Menlo Park, CA, USA, 5/2022. (oral)
8. **Materials Challenges in Alternative and Renewable Energy 2021 Virtual (MCARE 2021)**, D. Shin, W. Yeo, M. Kim, and J. W. Han, "Structure-Activity Relationship of VO_x/TiO_2 Catalysts for Mercury Oxidation: A DFT Study", online, USA, 7/2021. (poster)
9. **2019 AIChE Annual Meeting**, D. Shin, M. G. Jang, and J. W. Han, "Reducibility in the Catalytic Activity of CO Oxidizing Reactions on Pd Loaded Cu-Doped Ceria", Orlando, FL, USA, 11/2019. (poster)
10. **Materials Challenges in Alternative and Renewable Energy 2019 (MCARE2019)**, D. Shin and J. W. Han, "Density Functional Theory Study of the Preferential CO Oxidation on $\text{CeO}_2(111)$ under Rich H_2 Environment", Jeju, Korea, 8/2019. (poster)
11. **The 17th Korea-Japan Symposium on Catalysis (17KJSC)**, D. Shin, S. K. Sahoo, and J. W. Han, "Theoretical Investigation of Oxidative Methane Conversion on PdO/CeO_2 Catalyst", Jeju, Korea, 5/2019. (poster)
12. **The 20th Asian Workshop on First-Principles Electronic Structure Calculations (ASIAN-20)**, D. Shin and Y. -H. Kim, "Parallelization of the Higher-Order Finite Difference-Based Electronic Structure Calculation Code", Nanjing, China, 10/2017. (poster)
13. **NANO KOREA 2017**, D. Shin, J. Lee, J. I. Choi, and Y. -H. Kim, "Development of Magnetism in Armchair Graphene Nanoribbons with Edge Functionalizations: A First-Principles Study", Ilsan, Korea, 7/2017. (poster)

SOFTWARES & LIBRARIES

1. **CatDegUS** (Python, BoTorch) ([GitHub](#))
- Python module for Catalysts' Degradation navigated by Uncertainty Sampling
2. **pydrifts3D** (Python) ([GitHub](#))
- python code to convert the experimental raw spectra data from DRIFTS (Diffuse Reflectance Infrared Fourier Transform Spectroscopy) to three-dimensional plot

3. **SegrDNN** (Python, TensorFlow) ([GitHub](#))
 - Codes for closed-loop hyper-parameter tuning of DNN model using Bayesian optimization (BO) for the design of alloy catalysts
4. **PyCatRobin** (Python) ([GitHub](#))
 - Python module to analyze time-on-stream **Catalyst** testing results from Round **Robin** test
5. **MDUI (C)** ([GitHub](#))
 - from-scratch molecular dynamics (MD) program with graphic user interface (GUI)

TEACHING

1. **Teaching Assistant**
 - *Molecular Simulation for Chemical Engineers, Physical Chemistry, Winter Research Internship* – POSTECH
 - *Introductory Quantum Mechanics Simulation* – KAIST
2. **Tutoring Undergraduate Students**
 - *General Chemistry* – University of Seoul
 - *Summer/Winter Research Internship (Molecular Simulation, Machine Learning)* – POSTECH
3. **Mentoring**
 - 1) **Woonsuk Yeo** (from POSTECH; now a Ph.D. Candidate at Seoul National University)
 - Period: 11/2020-3/2023
 - Guidance on the research for VO_x/TiO₂ catalyst design for Hg oxidation
 - co-authored a publication; *ACS Catal.* 13 (2023) 3775-3787.
 - 2) **Hayoung Cho** (from Cooper Union; now a Quality Engineer at SK Battery America)
 - Period: 4/2022-8/2022
 - Guidance on supported metal catalyst optimization project using Bayesian optimization
 - 3) **Michael Mirabueno Albrechtsen** (from Technical University of Denmark)
 - Period: 2/2025-6/2025
 - Guidance on a project about comparability assessment of catalyst durability test results
 - co-authored a publication; to be submitted (2025).

SERVICE

1. **Reviewer**
 - *Molecular Catalysis, Korean Journal of Chemical Engineering*
2. **Acknowledgement** (designing and developing figures)
 - Universal prediction of strain footprints via simulation, statistics, and machine learning: low- Σ grain boundaries, *Acta Mater.* 211 (2021) 116850.
 - In situ Visualization of Cluster-mediated Oxidation Dynamics and Kinetics on Cu(111), submitted (2025). DOI: 10.26434/chemrxiv-2023-s2zwg-v2

TECHNICAL SKILLS

1. **Atomistic/Molecular Simulations**
 - Density functional theory (DFT) calculations (*VASP*, *SIESTA*),
 - Ab-initio thermodynamics approach to calculate Gibbs free energy diagram
 - Nudged elastic band (NEB) calculation (using *VTST Tools*)
 - Genetic algorithm (GA) for structural optimization of supported nanoparticle model (using *ASE*)
 - Catalyst surface modeling by *pymatgen* and *ASE*
 - Experience in programming basic molecular dynamics (MD) code based on *C*
2. **Programming**
 - *Python*, *Shell* script, experiences in *C*, *Java*, *Fortran*
 - Hands-on experience in parallel programming using *MPI* library
 - Project deployment using *GitHub*
 - Integrated Development Environment such as Visual Studio Code, PyCharm

3. Artificial Intelligence (AI)

- Neural network model training (using *keras*, *keras_tuner*, *scikit-learn*)
- Bayesian optimization, uncertainty sampling (using *GPy*, *GPyOpt*, *BoTorch*, *scikit-learn*)
- Interpretable AI (using *shap*), (sparse) principal component analysis (PCA) (using *scikit-learn*)

4. Scientific Visualization

- Atomic structure: *POV-Ray* (in combination with *ase-gui*), *blender*
- Experimental spectra: made a plotting tool for DRIFT spectra (<https://github.com/dongjae-shin/pydrifts3d>)
- *matplotlib*, *seaborn*

RESEARCH INTERESTS

1. Computational Design of Heterogeneous Catalysts via DFT and AI

- Elucidation of atomistic origins of activity/stability changes with respect to atomic modifications on heterogeneous catalysts; relevant reactions: exhaust emission control, e.g., oxidations of CO and Hg, syngas conditioning, e.g., water-gas shift (WGS), Power-to-Liquid, e.g., reverse water-gas shift reaction (RWGS)
- Development of design principles for durable catalysts
- Data-frugal design of experiments via Bayesian optimization (BO) to optimize synthetic condition for high-performance catalysts

2. Construction of Catalytic Data Infrastructure for AI Applications

- Data-frugal data sampling via uncertainty quantification for mapping feature-target relationship
- Development of data ontology to design AI-ready data representation
- Construction of FAIR-compliant cloud database
- Large-language model (LLM)-based assistant to make legacy data AI-ready

3. Development of Computational Tools for Computational and Experimental Researchers

- AI-aided acceleration of DFT calculation, e.g., AI-aided structural optimization of supported nanoparticle model
- Developed an open source code for the visualization of experimental spectral data (*pydrifts3d*)
- Statistical comparability assessment tool for time-on-stream catalyst testing results from multiple laboratories (*PyCatRobin*)