Dongjae Shin

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EDUCATION

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

EXPERIENCE

2/2024 –	**Postdoctoral Scholar**, SUNCAT Center for Interface Science and Catalysis, **SLAC National Accelerator Laboratory**, **Stanford University** Advisors: Kirsten T. Winther and Christopher J. Tassone	Menlo Park, United States
9/2023 – 1/2024	**Senior Researcher**, Department of Materials Science and Engineering, **SNU**[c]	Seoul, Korea
10/2018 – 2/2019	**Researcher**, Department of Chemical Engineering, **POSTECH**	Pohang, Korea
3/2018 – 3/2018	**Contract Research Scientist**, Applied Science Research Institute, **KAIST**	Daejeon, Korea
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 CO_2 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 CeO_2 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 VOx 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 H_2 on Low-Temperature Water-Gas Shift Reaction Activity of Pt/CeO_2 Catalyst by Forming CeO_2 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 Co_3O_4 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/TiO_2 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/CeO_2 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 Co_3O_4 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, NW, 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 $CeO_2(111)$ 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 **Cat**alysts' **Deg**radation navigated by **U**ncertainty **S**ampling
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)
   - **Py**thon module to analyze time-on-stream **Cat**alyst 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/TiO_2 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)