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EDUCATION

2/2019 – 8/2023	Ph.D. in Chemical Engineering, POSTECH Advisor: Prof. 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 ^a Advisor: Prof. 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 <i>Cum Laude</i> ; top honor in Chemical Engineering	Seoul, Korea

EXPERIENCE

9/2023 –	Postdoctoral Researcher , Department of Materials Science and Engineering, SNU ^b	Seoul, Korea
10/2018 – 2/2019	Researcher , Department of Chemical Engineering, POSTECH	Pohang, Korea
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	Teaching Undergraduate Students , School of General Education, University of Seoul (Subject: General Chemistry)	Seoul, Korea

PUBLICATIONS (†: equal contribution, *: corresponding author, parenthesis: published/latest year's IF)——— 17 papers including 9 first/co-first author papers and 2 submitted co-first author papers

- 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*, submitted (2023).
- Rh single-atom catalysts formed on defective CeO₂ surfaces with outstanding hydroformylation activity
 H. Lee†, **D. Shin**†, D. Oh†, B. Jeong, K. Y. Kim, C. Hur, J. W. Han*, and K. An*, submitted (2023).
- 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. (IF=4.6)
- 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. (IF=12.9)
Selected as a Supplementary cover
- 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. (IF=11.9) *Selected as a Back cover*

^a KAIST: Korea Advanced Institute of Science and Technology

^b SNU: Seoul National University

6. 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. (IF=12.9)
7. 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. (IF=12.9)
8. 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. (IF=9.4)
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. (IF=22.1)
10. 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). (IF=13.700)
Selected as a Supplementary cover
11. 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. (IF=7.392)
12. 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. (IF=13.084)
Selected as a Supplementary cover
13. 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. (IF=15.336)
14. 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. (IF=8.928)
15. 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. (IF=5.686)
Selected as a Front cover and Very Important Paper
16. 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. (IF=N/A)
17. 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. (IF=12.350)

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. **Best Poster Award**, NANO KOREA 2017, 7/2017
9. **4th Place in Team Contest**, The 8th KIAS CAC Summer School on Parallel and Scientific Computing, 6/2017
10. **Government Scholarship**, Ministry of Education, Science and Technology, 2016 – 2018, ~**29,000 USD**
11. **Encouragement prize**, 5th EDISON Software Utilization Contest hosted by KISTI, 3/2016
12. **Scholarship for Excellent Achievement**, University of Seoul, 2014 – 2015, ~**1,800 USD**
13. **University Development Fund Scholarship**, University of Seoul, 2014, ~**1,200 USD**
14. **Seoul Mayor's Scholarship for Excellent Achievement**, University of Seoul, 2010 – 2011, ~**7,200 USD**
15. **Academic Excellence Award**, University of Seoul, 1st semester 2011, 2nd semester 2010, 1st semester 2010

PATENTS

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 (application)

PRESENTATIONS (INTERNATIONAL)

1. **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)
2. **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)
3. **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)
4. **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)
5. **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/TiO₂ Catalysts for Mercury Oxidation: A DFT Study", online, USA, 7/2021. (poster)
6. **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)
7. **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 CeO₂(111) under Rich H₂ Environment", Jeju, Korea, 8/2019. (poster)
8. **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/CeO₂ Catalyst", Jeju, Korea, 5/2019. (poster)
9. **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)
10. **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)

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*)
- Experience in programming basic molecular dynamics (MD) code based on C

2. Programming

- *Python*, *Shell* script, experiences in *C*, *Java*, *Fortran*
- Experience in parallel programming using *MPI* library

3. Artificial Intelligence (AI)

- Neural network regression (using *keras*, *keras_tuner*, *scikit-learn*)
- Bayesian optimization (using *GPyOpt*)
- 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 Heterogeneous Catalysis

- Elucidation of atomistic origins of activity/stability changes with respect to atomic modifications in heterogeneous catalysts; relevant reactions: exhaust emission control (oxidations of CO and Hg, etc.) and hydrogen production (water-gas shift reaction)

2. Combination of Artificial Intelligence with Experimental Data

- Bayesian optimization of synthetic condition (1) for ex-solution catalyst using experimentally measured, and (2) for supported metal catalyst using experimental data from literature

3. Development of Tools for Computational and Experimental Researchers

- Relevant experience: development of AI-aided method for structural optimization of supported nanoparticle model (computational), making python code for the visualization of experimental spectra (experimental)

LIST OF REFEREES

1. Jeong Woo Han, Ph.D. (Advisor during Ph.D. program)

Associate Professor, Department of Materials Science and Engineering, Seoul National University (SNU), Seoul, Korea

Editor, *Molecular Catalysis*

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2. Hyunjoo Lee, Ph.D. (a corresponding author of my co-first author papers)

Professor, Department of Chemical and Biomolecular Engineering, Korea Advanced Institute of Science and Technology (KAIST), Daejeon, Korea

Associate Editor, *JACS Au*

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3. Kwangjin An, Ph.D. (Ph.D. committee member, a corresponding author of my co-first author papers)

Associate Professor, School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology (UNIST), Ulsan, Korea

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