Stanford



Dongjae Shin

Postdoctoral Scholar, Photon Science, SLAC

Bio

BIO

My current research focuses on the design of catalytic materials. My approaches to this topic include:

(1) First-principles calculation: using density functional theory (DFT), I have studied atomistic phenomena on catalytic surfaces with the purpose of developing materials with improved catalytic capability under the philosophy of rational design and high-throughput screening.

(2) AI-accelerated first-principles calculation: I have applied AI algorithms, e.g., evolutionary algorithm, Bayesian optimization, to the acceleration of computationally costly processes, enabling exploration of larger catalytic design space.

(3) AI-steered adaptive experimentation: I have applied active learning methods, e.g., uncertainty-based sampling, Bayesian optimization, to construct proxies of whole landscape of catalytic performance, or to perform multi-objective optimization. This is the brain of self-driving laboratory (SDL).

Applications include heterogeneous catalysis for exhaust emission control, hydrogen production, utilization of emission gas to realize carbon neutralization, and discovery of battery materials.

PROFESSIONAL EDUCATION

- M.S., Korea Advanced Institute of Science and Technology (KAIST) , Energy, Environment, Water and Sustainability (2018)
- Ph.D., Pohang University of Science and Technology (POSTECH) , Chemical Engineering (2023)

STANFORD ADVISORS

- Kirsten Winther, Postdoctoral Research Mentor
- Thomas Jaramillo, Postdoctoral Faculty Sponsor

LINKS

- Personal Site: https://dongjae-shin.github.io/
- Google Scholar: https://scholar.google.co.kr/citations?user=-9HK8-AAAAAJ&hl=en
- LinkedIn: https://www.linkedin.com/in/dongjae-shin-01095313a/?locale=en_US

Publications

PUBLICATIONS

- **Data as the Backbone of Artificial Intelligence: Insights from Heterogeneous Catalysis** *ACS CATALYSIS*
  Shin, D., Mahajan, R., Lian, Z., Heinlein, J., Cargnello, M., Tassone, C. J., Winther, K. T.
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- **Quantifying uncertainty in catalyst activity and deactivation during CO hydrogenation via round-robin testing for data-driven modelling** *NATURE CATALYSIS*
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- **Highly Durable Rh Single Atom Catalyst Modulated by Surface Defects on Fe-Ce Oxide Solid Solution.** *Angewandte Chemie (International ed. in English)*
  Kim, G., Choung, S., Hwang, J. E., Choi, Y., Kim, S., Shin, D., Han, J. W., Lee, H.
  2025; 64 (10): e202421218
- **Unmatched Redox Activity of the Palladium-Doped Indium Oxide Oxygen Carrier for Low-Temperature CO2 Splitting.** *ACS nano*
  Park, S., Oh, D., Jang, M. G., Seo, H., Kim, U., Ahn, J., Choi, Y., Shin, D., Han, J. W., Jung, W., Kim, I. D.
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- **Atomically dispersed Rh catalysts formed on defective CeO 2 surfaces with hydroformylation activity** *CHEMICAL ENGINEERING JOURNAL*
  Lee, H., Shin, D., Oh, D., Jeong, B., Kim, K., Hur, C., Han, J., An, K.
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- **Accelerated Structural Optimization for the Supported Metal System Based on Hybrid Approach Combining Bayesian Optimization with Local Search.** *Journal of chemical theory and computation*
  Bae, S., Shin, D., Kim, H., Han, J. W., Lee, J. M.
  2024; 20 (5): 2284-2296
- **Surface segregation machine-learned with inexpensive numerical fingerprint for the design of alloy catalysts** *MOLECULAR CATALYSIS*
  Shin, D., Choi, G., Hong, C., Han, J.
  2023; 541
- **Change in the Electronic Environment of the VO_XActive Center via Support Modification to Enhance Hg Oxidation Activity** *ACS CATALYSIS*
  Yeo, W., Shin, D., Kim, M., Han, J.
  2023; 13 (6): 3775-3787
- **Modulating the water gas shift reaction via strong interfacial interaction between a defective oxide matrix and exsolved metal nanoparticles** *JOURNAL OF MATERIALS CHEMISTRY A*
  Chen, H., Huang, R., Jang, M., Lim, C., Shin, D., Liu, Q., Yang, H., Chen, Y., Han, J.
  2022; 10 (47): 24995-25008
- **Role of an Interface for Hydrogen Production Reaction over Size- Controlled Supported Metal Catalysts** *ACS CATALYSIS*
  Shin, D., Huang, R., Jang, M., Choung, S., Kim, Y., Sung, K., Kim, T., Han, J.
  2022
- **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** *APPLIED CATALYSIS B-ENVIRONMENT AND ENERGY*
  Lee, J., Shin, D., Lee, E., Li, C., Kim, J., Han, J., Kim, D.
  2022; 305
- **Boosting Support Reducibility and Metal Dispersion by Exposed Surface Atom Control for Highly Active Supported Metal Catalysts** *ACS CATALYSIS*
  Jang, M., Yoon, S., Shin, D., Kim, H., Huang, R., Yang, E., Kim, J., Lee, K., An, K., Han, J.
  2022; 12 (8): 4402-4414
- **Universally characterizing atomistic strain via simulation, statistics, and machine learning: Low-angle grain boundaries** *ACTA MATERIALIA*
  Curnan, M. T., Shin, D., Saidi, W. A., Yang, J. C., Han, J.
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- **Facet-Dependent Mn Doping on Shaped Co₃O₄ Crystals for Catalytic Oxidation** *ACS CATALYSIS*
  Bae, J., Shin, D., Jeong, H., Choe, C., Choi, Y., Han, J., Lee, H.
  2021; 11 (17): 11066-11074

- **Structure-activity relationship of VO_x/TiO₂ catalysts for mercury oxidation: A DFT study** *APPLIED SURFACE SCIENCE*
  Shin, D., Kim, M., Han, J.
  2021; 552
- **Design of an Ultrastable and Highly Active Ceria Catalyst for CO Oxidation by Rare-Earth- and Transition-Metal Co-Doping** *ACS CATALYSIS*
  Kim, H., Shin, D., Jeong, H., Jang, M., Lee, H., Han, J.
  2020; 10 (24): 14877-14886
- **Controlling the Oxidation State of Pt Single Atoms for Maximizing Catalytic Activity** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*
  Jeong, H., Shin, D., Kim, B., Bae, J., Shin, S., Choe, C., Han, J., Lee, H.
  2020; 59 (46): 20691-20696
- **Oxidative Methane Conversion to Ethane on Highly Oxidized Pd/CeO₂ Catalysts Below 400 °C** *CHEMSUSCHEM*
  Kwon, G., Shin, D., Jeong, H., Sahoo, S., Lee, J., Kim, G., Choi, J., Kim, D., Han, J., Lee, H.
  2020; 13 (4): 677-681
- **Design of Ceria Catalysts for Low-Temperature CO Oxidation** *CHEMCATCHEM*
  Kim, H., Jang, M., Shin, D., Han, J.
  2020; 12 (1): 11-26
- **Highly Water-Resistant La-Doped Co₃O₄ Catalyst for CO Oxidation** *ACS CATALYSIS*
  Bae, J., Shin, D., Jeong, H., Kim, B., Han, J., Lee, H.
  2019; 9 (11): 10093-10100
- **Improved CO Oxidation via Surface Stabilization of Ceria Nanoparticles Induced by Rare-Earth Metal Dopants** *ACS APPLIED NANO MATERIALS*
  Noh, K., Kim, K., Kim, H., Shin, D., Han, J.
  2019; 2 (10): 6473-6481