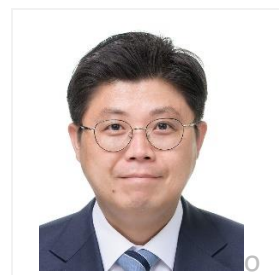


Curriculum Vitae

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EDUCATION

KAIST, Daejeon, Korea	Ph.D	Mater. Sci. & Eng.	2005
Hanyang University, Seoul, Korea	MS	Mater. Sci. & Eng.	2001
Hanyang University, Seoul, Korea	BS	Mater. Sci. & Eng.	1999

PROFESSIONAL ACTIVITIES

- Head, Computational Science Research Center, Korea Institute of Science and Technology (KIST), Korea, September 2020 to Present.
- Principal Research Scientist, KIST, Seoul, Korea, March 2017 to Present
- Senior Research Scientist, KIST, Seoul, Korea, June 2013 to February 2017
- Senior Research Scientist, Korea Research Institute of Standards and Science, Daejeon, Korea, February 2009 to May 2013
- Post-doctoral Scholar, California Institute of Technology, USA, October 2005 to January 2009

AWARD AND HONORS

- KIST Young Fellow, 2018

RESEARCH INTERESTS

- Artificial intelligence & machine-learning based material design
- Self-driving lab for material development based AI robots
- Multi-scale simulation for material design

MAIN SCIENTIFIC PUBLICATION (Total 109 SCI papers)

- M. J. Banisalman, M.-C. Kim, and S. S. Han, Origin of Enhanced Ammonia Synthesis on Ru-Co Catalysts Unraveled by Density Functional Theory, ACS Catalysis 12, 1090-1097 (2022).
- B. C. Yeo, H. Nam, H. Nam, M.-C. Kim, H. W. Lee, D. Kim, K.-Y. Lee, S. Y. Lee, and S. S. Han, High-Throughput Computational-Experimental Screening Protocol for the Discovery of Bimetallic Catalysts, npj Computational Materials 7, 137 (2021).
- H. W. Lee, H. Nam, G.-H. Han, Y.-H. Cho, B. C. Yeo, M.-C. Kim, D. Kim, K.-Y. Lee, S.Y. Lee, S. S. Han, Solid-Solution Alloying of Immiscible Pt and Au Boosts Catalytic Performance for Direct H₂O₂ Synthesis, Acta Materialia 205, 1165363 (2021).
- L.C.O. Tiong, J. Kim, S. S. Han, D. Kim, Identification of Crystal Symmetry from Noisy Diffraction Patterns by A Shape Analysis and Deep Learning, npj Computational Materials 6, 196 (2020).

- M.-C. Kim, H. Nam, J. Choi, H. S. Kim, H. W. Lee, D. Kim, J. Kong, S. S. Han, S. Y. Lee, and H. S. Park, Hydrogen Bonding-Mediated Enhancement of Bioinspired Electrochemical Nitrogen Reduction on Cu_{2-x}S Catalysts, *ACS Catalysis* 10, 10577-10584 (2020).
- M. Kim, B. C. Yeo, Y. Park, H. M. Lee, S. S. Han, and D. Kim, Artificial Intelligence to Accelerate the Discovery of N_2 Electroreduction Catalysis, *Chemistry of Materials* 32, 709-720 (2020).
- D. Kim, H. Nam, Y. H. Cho, B. C. Yeo, S.-H. Cho, J.-P. Ahn, K.-Y. Lee, S. Y. Lee, and S. S. Han, Unlocking the Potential of Nanoparticles Composed of Immiscible Elements for Direct H_2O_2 Synthesis, *ACS Catalysis* 9, 8702-8711 (2019).
- S.-J. Pai and S. S. Han, $\text{S}_\text{E}2$ Reaction in Non-Carbon System: Metal Halide Catalysis for Dehydrogenation of Ammonia Borane, *Proceedings of the National Academy of Science, USA* 114, 13625-13630 (2017)

PATENTS

- Pending: 43 (Korea, USA, Europe, China)
- Registered: 20 (Korea, USA, Japan)

TECHNOLOGY TRANSFER

- Slab graph convolution neural network for catalysis design, Virtual Lab Co. Ltd., 2021