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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

- Principal Research Scientist, Korea Institute of Science and Technology (KIST), Korea, March 2017 to Present
- Senior Research Scientist, KIST, Korea, June 2013 to February 2017
- Senior Research Scientist, Korea Research Institute of Standards and Science, Korea, February 2009 to May 2013
- Post-doctoral Scholar, Dept. of Chemistry, California Institute of Science and Technology, USA, October 2005 to January 2009

AWARD AND HONORS

- KIST Young Fellow, KIST, May 2018

MAIN SCIENTIFIC PUBLICATION

- B. C. Yeo, D. Kim, C. Kim, and S. S. Han, “Pattern Learning Electronic Density of States”, Scientific Reports 9 (2019) 5829(1)-(10).
- S. –Y. Kim, H. W. Lee, S.-J. Pai, and S. S. Han, “Activity, Selectivity, and Durability of Ruthenium Nanoparticle Catalysts for Ammonia Synthesis by Reactive Molecular Dynamics Simulation: The Size Effect”, ACS Applied Materials & Interfaces 10 (2018) 26188-26194.
- S.-J. Pai and S. S. Han, “S_E2 Reaction in Non-Carbon System: Metal Halide Catalysis for Dehydrogenation of Ammonia Borane”, Proceedings of the National Academy of Sciences, U.S.A. 114 (2017) 13625-13630.
- K.-S. Yun, S.-J. Pai, B.-C. Yeo, K.-R. Lee, S.-J. Kim, and S. S. Han, “Simulation Protocol for Prediction of a Solid-Electrolyte Interphase on the Silicon-Based Anodes of a Lithium-Ion Battery: ReaxFF Reactive Force Field”, Journal of Physical Chemistry Letters 8 (2017) 2812-2818.
- D. H. Seo, H. Shin, K. Kang, H. Kim, and S. S. Han, “First-Principles Design of Hydrogen Dissociation Catalysts Based on Isoelectronic Metal Solid Solutions”, Journal of Physical Chemistry Letters 5 (2014) 4285-4290.

RESEARCH INTERESTS

- Design of novel metallic catalysts for H2O2 direct synthesis and NH3 synthesis by first-principles calculations
- Multiscale simulations on gas storage and separation in porous materials (e.g., MOFs and zeolites)
- Atomistic and quantum simulations for development of novel battery materials
- Development of reactive force field (ReaxFF) to predict formation/dissociation of chemical bonds in large-scale systems
- Development of machine-learning techniques for accelerated material design