

Sang Soo Han

Head, Dr.

Computational Science Research Center, Korea Institute of Science and Technology (KIST), Korea

Curriculum Vitae



● Educational Background & Professional Experience

2020.9–Present	Head, Computational Science Research Center, KIST
2017.3–Present	Principal Research Scientist, KIST
2013.6–2017.2	Senior Research Scientist, KIST
2009.2–2013.5	Senior Research Scientist, Korea Research Institute of Standards and Science (KRISS)
2005.10–2009.1	Post-doctoral Scholar, Chemistry, California Institute of Technology
2001.3–2005.2	Ph. D, Materials Science and Engineering, KAIST
1999.3–2001.2	MS, Materials Science and Engineering, Hanyang University
1995.3–1999.2	BS, Materials Science and Engineering, Hanyang University

● Research Interests

Artificial intelligence & machine-learning based materials design, Self-driving lab for materials discovery, Multi-scale simulation for materials design

● Publications

1. N. Kim, H. J. Yoo, D. Kim, H. Lee, C. S. Hong, and S. S. Han*, SPACESHIP: Autonomous Mapping of Hardware-Dependent Synthesizable Space in Solution-Phase Gold Nanomaterials, J. Am. Chem. Soc., 2026.
2. J.-G. Lee, J. W. Choi, S. Kim, W. Zhang, H. Shin, J.-H. Kim, E. H. Sargent, S. S. Han*, J. M. Kim*, M.-J. Choi*, Ligand-Driven Tuning of Adsorption Energy in Nanocrystals for High-Performance H₂O₂ Electrosynthesis, J. Am. Chem. Soc. 2026.
3. J. S. Lee, S. Kim, S.-H. Kim, J.-H. Baek, C. Li, R. Guan, B.J. Jiang, G.-F. Han, S. S. Han*, J.-B. Baek*, Mechanochemical Ammonia Synthesis Enhanced by Silicon Nitride as a Defect-Inducing Physical Promoter, Nature Communications, 2025.
4. H. J. Yoo, K.-Y. Lee, D. Kim*, and S. S. Han*, OCTOPUS: operation control system for task optimization and job parallelization via a user-optimal scheduler, Nature Communications, 2024.
5. H. J. Yoo, N. Kim, H. Lee, D. Kim, L.C.O. Tiong, H. Nam, C. Kim, S. Y. Lee, K.-Y. Lee*, D. Kim*, and S. S. Han*, Bespoke Metal Nanoparticle Synthesis at Room Temperature and Discovery of Chemical Knowledge on Nanoparticle Growth Via Autonomous Experimentation, Advanced Functional Materials, 2024.