

Sang Soo Han

*Computational Science Research Center
Korea Institute of Science and Technology (KIST)
5 Hwarangro 14-gil, Seongbuk-gu, Seoul 02792, Republic of Korea
Tel: +82-2-958-5441; Fax: +82-2-958-5451; sangsoo@kist.re.kr
Webpage: <https://sites.google.com/site/sangsookist/home>*

PERSONAL INFORMATION:

Born June 5, 1976, Jeju city, Republic of Korea

EDUCATION:

- Ph. D. in Material Science and Engineering, KAIST, Daejeon, Korea (2005. 02)
*Dissertation title: Hydrogen Storage Properties of Carbon Nanotubes and Boron Nitride Nanotubes: Density Functional Theory and Reactive Force Field Studies
(Advisor: Prof. Hyuck Mo Lee)*
- M.S. in Mater. Sci. and Eng., Hanyang University, Seoul, Korea (2001. 02)
*Dissertation title: Development of Composite Metal Hydride Alloy of Mg-Ti-Ni System for the Ni-MH Battery by Mechanical Alloying
(Advisor: Prof. Kyung Sub Lee)*
- B.S. in Mater. Sci. and Eng., Hanyang University, Seoul, Korea (1999. 02)

RESEARCH EXPERIENCES:

- Head of Computational Science Research Center, KIST, Seoul, Korea (2020. Sep. ~ Present)
- Principal Research Scientist, KIST, Seoul, Korea (2017. Mar. ~ Present)
- Senior Research Scientist, KIST, Seoul, Korea (2013. Jun. ~ 2017. Feb.)
- Senior Research Scientist, Korea Research Institute of Standards and Science (KRISS), Daejeon, Korea (2009. Feb. ~ 2013. May)
- Post-doctoral Scholar at Department of Chemistry (*Advisor: Prof. W. A. Goddard III*), California Institute of Technology, CA, USA (2005. Oct. ~ 2009. Jan.)
- Post-doctoral Researcher at Applied Science Research Institute, KAIST, Daejeon, Korea (2005. Mar. ~ 2006. Nov.)

PUBLICATIONS (SCI): (* Corresponding author)

1. S. S. Han*, N. H. Goo, W. T. Jeong, and K. S. Lee, “Synthesis of Composite Metal Hydride Alloy of A₂B and AB Types by Mechanical Alloying”, *J. Power Sources*, 92 (2001) 157-162.
2. S. S. Han*, H. Y. Lee, N. H. Goo, W. T. Jeong, and K. S. Lee, “Improvement of Electrode Performances of Mg₂Ni by Mechanical Alloying”, *J. Alloys and Compounds*, 330-332 (2002) 841-845.
3. S. I. Park, S. S. Han, H. G. Kim, J. K. Park, and H. M. Lee*, “Three-Dimensional Monte-Carlo Simulation of Grain Growth in Pt-Co Thin Film”, *J. Electronic Materials*, 31 (2002) 965-971.
4. S. S. Han and H. M. Lee*, “Molecular Dynamics Simulation of Zigzag Single-Walled Carbon Nanotube Closing Mechanisms”, *Metals and Materials International*, 9 (2003) 99-105.
5. S. S. Han*, N. H. Goo, and K. S. Lee, “Effects of Sintering on Composite Metal Hydride Alloy of Mg₂Ni and TiNi Synthesized by Mechanical Alloying”, *J. Alloys and Compounds*, 360 (2003) 243-249.
6. S. S. Han, K. S. Lee, and H. M. Lee*, “Nucleation Mechanism of Carbon Nanotubes”, *Chemical Physics Letter*, 383 (2004) 321-325.
7. S. S. Han and H. M. Lee*, “Study on Cap Closure Mechanism of Single-Walled Carbon Nanotubes by Molecular Dynamics”, *Material Transaction, JIM*, 45 (2004) 1437-1441.
8. T. Y. Kim, S. S. Han, and H. M. Lee*, “Nanomechanical Behavior of β-SiC Nanowire in Tension: Molecular Dynamics Simulations”, *Material Transaction, JIM*, 45 (2004) 1442-1449.
9. S. S. Han and H. M. Lee*, “Adsorption Properties of Hydrogen on the (10,0) Single-Walled Carbon Nanotube through Density Functional Theory”, *Carbon*, 42 (2004) 2169-2177.
10. S. S. Han, J. K. Kang, A. C. T. van Duin, W. A. Goddard III, and H. M. Lee*, “Liquefaction of H₂ Molecules upon Exterior Surfaces of Carbon Nanotube Bundles”, *Applied Physics Letter*, 86 (2005) 203108.
11. S. S. Han, A. C. T. van Duin, W. A. Goddard III, and H. M. Lee*, “Optimization and Application for Lithium Parameters of Reactive Force Field, ReaxFF”, *J. Physical Chemistry A*, 109 (2005) 4575-4582.
12. K. S. Han, H. S. Kim, M. S. Song, M. S. Park, S. S. Han, J. Y. Lee, J. K. Kang*, and Y. K. Kim, “Atmospheric-Pressure Plasma Treatment to Modify Hydrogen Storage Properties of Multi-Walled Carbon Nanotubes”, *Applied Physics Letter*, 86 (2005) 263105.
13. S. S. Han, J. K. Kang, H. M. Lee*, A. C. T. van Duin, and W. A. Goddard III. “Theoretical Studies on Interaction of Hydrogen with Single-Walled Boron Nitride Nanotube. I. The Reactive Force Field ReaxFF_{HBN} Development”, *J. Chemical Physics*, 123 (2005) 114703. [selected for the October 3, 2005 issue of Virtual Journal of Nanoscale Science & Technology]
14. S. S. Han, J. K. Kang, H. M. Lee*, A. C. T. van Duin, and W. A. Goddard III. “Theoretical Studies on Interaction of Hydrogen with Single-Walled Boron Nitride Nanotube. II. Collision, storage and adsorption”, *J. Chemical Physics*, 123 (2005) 114704.
15. S. S. Han, S. H. Lee, J. K. Kang, and H. M. Lee*, “High Coverage of Hydrogen on a (10,0) Single-Walled Boron Nitride Nanotube”, *Physical Review B*, 72 (2005) 113402.
16. S. S. Han, H. S. Kim, K. S. Han, J. Y. Lee, H. M. Lee, J. K. Kang*, S. I. Woo, A. C. T. van Duin, and W. A. Goddard III, “Nanopores of Carbon Nanotubes as Practical Hydrogen Storage Media”, *Applied Physics Letters*, 87 (2005) 213113. [selected for the November 28, 2005 issue of Virtual Journal of Nanoscale Science &

Technology and introduced in R&D FOCUS, THE FUEL CELL REVIEW, volume 2, Issue 6, Dec/Jan 2006]

17. S. S. Han, W. -Q. Deng, and W. A. Goddard III*, "Improved Designs of Metal Organic Frameworks for Hydrogen Storage", *Angewandte Chemie International Edition*, 46 (2007) 6289-6292. (Chosen as a "Hot Paper")
18. S. S. Han and W. A. Goddard III*, "Li-Doped Metal-Organic Frameworks for High Hydrogen Storage at Ambient Temperature", *Journal of the American Chemical Society*, 129 (2007) 8422-8423.
19. S. S. Han and W. A. Goddard III*, "Metal Organic Framework Provides Large Negative Thermal Expansion", *Journal of Physical Chemistry C*, 111 (2007) 15185-15191.
20. S. H. Lee, S. S. Han, J. K. Kang, J. H. Ryu, and H. M. Lee*, "Phase Stability of Pt Nanoclusters and the Effect of a (0001) Graphite Surface through Molecular Dynamics Simulation", *Surface Science*, 602 (2008) 1433-1439.
21. S. S. Han, H. Furukawa, O. M. Yaghi*, and W. A. Goddard III*, "Covalent Organic Frameworks as Exceptional Hydrogen Storage Materials", *Journal of the American Chemical Society*, 130 (2008) 11580-11581.
22. S. S. Han and W. A. Goddard III*, "High H₂ Uptake of Hexagonal Metal-Organic Frameworks from First-Principles Based Grand Canonical Monte-Carlo Simulations", *Journal of Physical Chemistry C*, 112 (2008) 13431-13436.
23. A. C. T. van Duin, B. Merinov, S. S. Han, C. O. Dorso, and W. A. Goddard III*, "ReaxFF Reactive Force Field for the Y-Doped BaZrO₃ Proton Conductor with Applications to Diffusion Rates for Multigranular Systems", *Journal of Physical Chemistry A*, 112 (2008) 11414-11422.
24. S. S. Han, J. L. Mendoza-Cortés, and W. A. Goddard III*, "Recent Advances on Theory and Simulation of H₂ Storage in Metal-Organic Frameworks and Covalent-Organic Frameworks", *Chemical Society Reviews*, 38 (2009) 1460-1476. (Invited).
25. D. H. Kim*, J. H. Yoon, S. S. Han, K. S. Lee, J. S. Jang, S. H. Choi, D.-K. Choi, S.-J. Kim, Y. K. Sun, and K. S. Lee, "High Electrochemical Li Intercalation in Titanate Nanotubes", *Journal of Physical Chemistry C*, 113 (2009) 14034-14039.
26. S. S. Han* and S. S. Jang, "A hydrogen storage nanotank: lithium-organic pillared graphites", *Chemical Communications*, (2009) 5427-5429.
27. H. Y. Kim, S. S. Han, J. H. Ryu, and H. M. Lee*, "Balance in Adsorption Energy of Reactants Steers CO Oxidation Mechanism of Ag₁₃ and Ag₁₂Pd₁ Nanoparticles: Association Mechanism versus Carbonate Mediated Mechanism", *Journal of Physical Chemistry C*, 114 (2010) 3156-3160.
28. S. S. Han,* T. H. Yu, B. Merinov, A. C. T. van Duin, R. Yazami, and W. A. Goddard III*, "Unraveling Structural Models of Graphite Fluorides by Density Functional Theory Calculations", *Chemistry of Materials*, 22 (2010) 2142-2154.
29. S. S. Han,* S. -H. Choi, and W. A. Goddard III, "Zeolitic Imidazolate Frameworks as H₂ Adsorbents: Ab-Initio Based Grand Canonical Monte-Carlo Simulation", *Journal of Physical Chemistry C*, 114 (2010) 12039-12047.
30. S. S. Han,* S. -H. Choi, and A. C. T. van Duin, "Molecular Dynamics Simulations of Stability of Metal-Organic Frameworks against H₂O Using ReaxFF Reactive Force Field", *Chemical Communications*, 46 (2010) 5713-5715.

31. J. L. Mendoza-Cortés, S. S. Han, H. Furukawa, O. M. Yaghi*, and W. A. Goddard III*, “Adsorption Mechanism and Uptake of Methane in Covalent-Organic Frameworks: Theory and Experiment”, *Journal of Physical Chemistry A*, 114 (2010) 10824-10833.
32. S. S. Han*, S. -H. Choi, and W. A. Goddard III,* “Improved H₂ Storage in Zeolitic Imidazolate Frameworks Using Li⁺, Na⁺, and K⁺ Dopants, with an Emphasis of Delivery H₂ Uptake”, *Journal of Physical Chemistry C*, 115 (2011) 3507-3512.
33. J. H. Ryu, S. S. Han, D. H. Kim, G. Henkelman, and H. M. Lee,* “Ligand- Induced Structural Evolution of Pt₅₅ Nanoparticles: Amine versus Thiol”, *ACS Nano*, 5 (2011) 8515-8522.
34. S. S. Han*, H. Kim, and N. Park,* “Effect of Shuttling Catalyst on the Migration of Hydrogen Adatoms: A Strategy for the Facile Hydrogenation of Graphene”, *Journal of Physical Chemistry C*, 115 (2011) 24696-24701.
35. D. Kim, D. H. Jung, K. -H. Kim, H. Guk, S. S. Han, K. Choi,* S. -H. Choi,* “Pillared Covalent Organic Frameworks with Balanced Volumetric and Gravimetric Hydrogen Uptake”, *Journal of Physical Chemistry C*, 116 (2012) 1479-1484.
36. J. L. Mendoza-Cortés, S. S. Han, and W. A. Goddard III,* “High H₂ Uptake in Li-, Na-, and K-Metalated Covalent Organic Frameworks and Metal Organic Frameworks at 298 K”, *Journal of Physical Chemistry A*, 116 (2012) 1621-1631.
37. J. Park, H. Kim, S. S. Han, and Y. Jung,* “Tuning Metal-Organic Frameworks with Open-Metal Sites and Its Origin for Enhancing CO₂ Affinity by Metal Substitution”, *Journal of Physical Chemistry Letters*, 3 (2012) 826-829.
38. S. S. Han, H. Jung, D. H. Jung,* S. -H. Choi, and N. Park,* “Stability of Hydrogenation States of Graphene and Conditions for Hydrogen Spillover”, *Physical Review B*, 85 (2012) 155408(1)-155408(5).
39. S. S. Han*, D. Kim, D. H. Jung, S. Cho, S. -H. Choi, and Y. Jung,* “Accurate Ab Initio-Based Force Field for Predictive CO₂ Uptake Simulations in MOFs and ZIFs: Development and Applications for MTV-MOFs”, *Journal of Physical Chemistry C*, 116 (2012) 20254-20261.
40. S. S. Han*, D. H. Jung, and J. Heo,* “Interpenetration of Metal Organic Frameworks for Carbon Dioxide Capture and Hydrogen Purification: Good or Bad?”, *Journal of Physical Chemistry C*, 117 (2013) 71-77.
41. D. Kim, D. H. Jung, H. Guk, S. S. Han, N. Park, K. Choi,* and S.-H. Choi,* “Theoretical Study on Porphyrin Based Covalent Organic Polyhedra as a Hydrogen Storage”, *International Journal of Hydrogen Energy*, 38 (2013) 6234-6240.
42. S. C. Yeo, S. S. Han, and H. M. Lee,* “Adsorption, Dissociation, and Diffusion of N₂ on and in BCC Fe: First-principles Calculations”, *Physical Chemistry and Chemical Physics*, 15 (2013) 5186-5192.
43. D. Shin, H. Jung, S. S. Han, C. H. Choi, H. Lee, and N. Park,* “Microscopic Nature of Mobile Fluoride Anions on sp² Carbon Surfaces”, *Chemical Physics Letters*, 570 (2013) 85-89.
44. S. S. Han*, D. H. Jung, S.-H. Choi, and J. Heo,* “Lithium-Functionalized Metal Organic Frameworks that Show >10 wt% H₂ Uptake at Ambient Temperature”, *ChemPhysChem*, 14 (2013) 2698-2703.
45. J. Joo, H. Kim,* and S. S. Han*, “Volume Shrinkage of Metal Organic Framework Host Induced by the Dispersive Attraction of Guest Gas Molecules”, *Physical Chemistry Chemical Physics*, 15 (2013) 18822-18826. (*Back cover selected*)

46. D. Odkhuu, D. H. Jung, H. Lee, S. S. Han, S.-H. Choi, R. S. Ruoff, and N. Park*, “Negatively Curved Carbons as the Anode for Lithium Ion Batteries”, *Carbon*, 66 (2014) 39-47.
47. W. R. Lee, S. Y. Hwang, D. W. Ryu, K. S. Lim, S. S. Han, D. Moon, J. Choi, and C. S. Hong*, “Diamine-Functionalized Metal-Organic Framework: Exceptionally High CO₂ Capacities from Ambient Air and Flue Gas, Ultrafast CO₂ Uptake Rate, and Adsorption Mechanism”, *Energy & Environmental Science*, 7 (2014) 744-751.
48. D. H. Chung, H. Guk, D. Kim, S. S. Han, N. Park, K. Choi, and S.-H. Choi*, “The effect of the stacking fault on the diffusion of chemisorbed hydrogen atoms inside few-layered graphene”, *RSC Advances*, 4 (2014) 9223-9228.
49. J. Joo, H. Kim,* and S. S. Han*, “Reply to the ‘Comment on “Volume shrinkage of metal organic framework host induced by the dispersive attraction of guest gas molecules” by F.-X. Coudert, A. H. Fuchs, and A. V. Neimark’ ”, *Physical Chemistry Chemical Physics*, 16 (2014) 4396-4398.
50. S. C. Yeo, S. S. Han, and H. M. Lee*, “Mechanistic Investigation of the Catalytic Decomposition of Ammonia (NH₃) on an Fe(100) Surface: A DFT Study”, *Journal of Physical Chemistry C*, 118 (2014) 5309-5316.
51. L.-M. Yang,* G.-Y. Fang, J. Ma, and S. S. Han, “Band Gap Engineering of Paradigm MOF-5”, *Crystal Growth & Design*, 14 (2014) 2532-2541.
52. 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) 1819-1824.
53. R. P. Hardikar, D. Das, S. S. Han, K.-R. Lee, and A. K. Singh*, “Boron Doped Defective Graphene as a Potential Anode Material for Li-ion Batteries”, *Physical Chemistry Chemical Physics* 16 (2014) 16502-16508.
54. D. Das, S. S. Han, K.-R. Lee, and A. K. Singh*, “Pressure Induced Manifold Enhancement of Li-Kinetics in FCC Fullerene”, *Physical Chemistry Chemical Physics* 16 (2014) 21688-21693.
55. J. Jeon, Y. C. Park, S. S. Han, W. A. Goddard III, Y. S. Lee, and H. Kim*, “Rapid Dye Regeneration Mechanism of Dye-Sensitized Solar Cells”, *Journal of Physical Chemistry Letters* 5 (2014) 4285-4290.
56. H. Jung, M. Lee, B. C. Yeo, K.-R. Lee, and S. S. Han*, “Atomistic Observation of the Lithiation and Delithiation Behaviors of Silicon Nanowires using Reactive Molecular Dynamics Simulations”, *Journal of Physical Chemistry C* 119 (2015) 3447-3455.
57. P. Srivastava, K. P. S. S. Hembram, H. Mizuseki, K.-R. Lee, S. S. Han*, and S. Kim*, “Tuning the Electronic and Magnetic Properties of Phosphorene by Vacancies and Adatoms”, *Journal of Physical Chemistry C* 119 (2015) 6530-6538.
58. W. R. Lee, L.-M. Yang, D. W. Ryu, K. S. Lim, J. H. Song, S. S. Han, D. Moon, and C. S. Hong*, “Exceptional CO₂ Working Capacity in a Heterodiamine-Grafted Metal-Organic Framework”, *Chemical Science* 6 (2015) 3697-3705.
59. K. P. S. S. Hembram, H. Jung, B. C. Yeo, S. J. Pai, S. Kim, K. -R. Lee, and S. S. Han*, “Unraveling the Atomistic Sodiation Mechanism of Black Phosphorus for Sodium Ion Batteries by First-Principles Calculations”, *Journal of Physical Chemistry C* 119 (2015) 15041-15046.
60. S. J. Pai, B. C. Yeo, and S. S. Han*, “Development of the ReaxFF_{CBN} Reactive Force Field for the Improved Design of Liquid CBN Hydrogen Storage Materials”, *Physical Chemistry Chemical Physics* 18 (2016) 1818-

61. S. H. Park, H. M. Park, S. S. Han, S. Y. Han, and J. Y. Song*, “Solid-solution alloying of immiscible metals at the nanoscale: Ir and Au”, *RSC Advances* 6 (2016) 3210-3212.
62. H. Guk, D. Kim, S.-H. Choi, D. H. Chung,* and S. S. Han, “Themostable Artificial Solid-Electrolyte Interface Layer Covalently Linked to Graphite for Lithium Ion Battery: Molecular Dynamics Simulations”, *Journal of Electrochemical Society* 163 (2016) A917-A922.
63. G. Y. Yoo, W. R. Lee, H. Jo, J. Park, J. H. Song, K. S. Lim, D. Moon, J. Lim, S. S. Han,* Y. Jung,* and C. S. Hong*, “Adsorption of Carbon Dioxide on Unsaturated Metal Sites in M₂(dobpdc) Frameworks with Exceptional Structural Stability and Relation between Lewis Acidity and Adsorption Enthalpy”, *Chemistry – A European Journal* 22 (2016) 7444-7451.
64. H. Choi, D. Shin, B. C. Yeo, T. Song, S. S. Han, N. Park, and S. Kim, “Simultaneously Controllable Doping Sites and the Activity of a W-N Co-Doped TiO₂ Photocatalyst”, *ACS Catalysis* 6 (2016) 2745-2753.
65. M. J. Park, J. H. Lee, K. P. S. S. Hembram, K.-R. Lee, S. S. Han, C. W. Yoon, S.-W. Nam, and J. Y. Kim*, “Oxygen Reduction Electrocatalysts Based on Coupled Iron Nitride Nanoparticles with Nitrogen-Doped Carbon”, *Catalysts* 6 (2016) 86(1)-(11).
66. K. P. S. S. Hembram, H. Jung, B. C. Yeo, S. J. Pai, H. J. Lee, K.-R. Lee, and S. S. Han* , “A Comparative First-Principles Study on the Lithiation, Sodiation, and Magnesiation of Black Phosphorus for Li-, Na-, and Mg-Ion Batteries”, *Physical Chemistry Chemical Physics* 18 (2016) 21391-21397.
67. B. C. Yeo, D. Kim, H. Kim, S. S. Han*, “High-Throughput Screening to Investigate the Relationship Between the Selectivity and Working Capacity of Porous Materials for Propylene/Propane Adsorptive Separation”, *Journal of Physical Chemistry C* 120 (2016) 24224-24230.
68. H. Jung, B. C. Yeo, K.-R. Lee, and S. S. Han*, “Atomistics of the Lithiation of Oxidized Silicon (SiO_x) Nanowires in Reactive Molecular Dynamics Simulations”, *Physical Chemistry Chemical Physics* 18 (2016) 32078-32086.
69. H. Jo, N. W. Kim, H. Jung, K. S. Lim, W. R. Lee, D. W. Kang, H. Lee, J. G. Seo, H. Jin, D. Moon, S. S. Han, and C. S. Hong*, “Fine-Tuning of the Carbon Dioxide Capture Capability of Diamine-Grafted MOF Adsorbents via Amine Functionalization”, *ChemSusChem* 10 (2017) 541-550. (19)
70. M.-g. Seo, H. J. Kim, S. S. Han, and K.-Y. Lee*, “Direct Synthesis of Hydrogen Peroxide from Hydrogen and Oxygen Using Tailored Pd Nanocatalysts: A Review of Recent Findings”, *Catalysis Surveys from Asia* 21 (2017) 1-12.
71. M.-g. Seo, H. J. Kim, S. S. Han, and K.-Y. Lee*, “Effect of Shell Thickness of Pd core-porous SiO₂ Shell Catalysts on Direct Synthesis of H₂O₂ from H₂ and O₂”, *Journal of Molecular Catalysis A: Chemical* 426 (2017) 238-243.
72. D. Kim, B. C. Yeo, D. Shin, H. Choi, S. Kim, N. Park, and S. S. Han*, “Dissimilar Anisotropy of Electron Versus Hole Bulk Transport in Anatase TiO₂: Implications for Photocatalysis”, *Physical Review B* 95 (2017) 045209(1)-(6).
73. G.-H. Han, M.-g. Seo, Y.-H. Cho, S. S. Han, and K.-Y. Lee*, “Highly Dispersed Pd Catalysts Prepared by a Sonochemical Method for the Direct Synthesis of Hydrogen Peroxide”, *Journal of Molecular Catalysis A:*

Chemical 429 (2017) 43-50.

74. S. Khan, H. Cho, D. Kim, S. S. Han, K. H. Lee, S.-H. Cho*, T. Song*, and H. Choi*, “Defect Engineering toward Strong Photocatalysis of Nb-doped Anatase TiO₂: Computational Predictions and Experimental Verifications”, *Applied Catalysis B: Environmental* 206 (2017) 520-530.
75. X. Y. Liu, S. J. Pai, and S. S. Han*, “ReaxFF Molecular Dynamics Simulations of Water Stability of Interpenetrated Metal-Organic Frameworks”, *Journal of Physical Chemistry C* 121 (2017) 7312-7318.
76. M.-g. Seo, D.-W. Lee*, S. S. Han, and K.-Y. Lee*, “Direct Synthesis of Hydrogen Peroxide from Hydrogen and Oxygen over Mesoporous Silica-Shell-Coated, Palladium-Nanocrystal-Grafted SiO₂ Nanobeads”, *ACS Catalysis* 7 (2017) 3039-3048.
77. R. Kanagaraj, Y.-S. Nam, S. J. Pai, S. S. Han, and K.-B. Lee*, “Highly Selective and Sensitive Detection of Cr⁶⁺ Ions Using Size-Specific Label-Free Gold Nanoparticles”, *Sensors and Actuators B: Chemical* 251 (2017) 683-691.
78. 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. ([†]Equally contributed)
79. D. Das, R. Hardikar, S. S. Han, K.-R. Lee, and A. Singh*, “Monolayer BC₂: An Ultrahigh Capacity Anode Material for Li Ion Batteries”, *Physical Chemistry Chemical Physics* 19 (2017) 24230-24239.
80. S. Song,[†] D. Kim,[†] H. M. Jang,* B. C. Yeo, S. S. Han, C. S. Kim, and J. F. Scott, “ β -CuGaO₂ as a Strong Candidate Material for Efficient Ferroelectric Photovoltaics”, *Chemistry of Materials* 29 (2017) 7596-7603. ([†]Equally contributed)
81. B. C. Yeo,[†] H. Jung,[†] H. W. Lee, K.-S. Yun, H. Kim, K.-R. Lee, and S. S. Han*, “Atomistic Simulation Protocol for Improved Design of Si-O-C Hybrid Nanostructures as Li-Ion Battery Anodes: ReaxFF Reactive Force Field”, *Journal of Physical Chemistry C* 121 (2017) 23268-23275. ([†]Equally contributed).
82. S. Seo, B. C. Yeo, S. S. Han, C. M. Yoon, J. Y. Yang, J. Yoon, C. Yoo, H.-j. Kim, Y.-b. Lee, S. J. Lee, J.-M. Myoung, H.-B.-R. Lee, W.-H. Kim, I.-K. Oh*, and H. Kim*, “Reaction Mechanism of Area-Selective Atomic Layer Deposition for Al₂O₃ Nanopatterns”, *ACS Applied Materials & Interfaces* 9 (2017) 41607-41617.
83. 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.
84. Y. Horbatenko, D. Shin, S. S. Han, and N. Park*, “Excitation-driven non-thermal conversion of few-layer graphenes into sp³-bonded nanofilms”, *Chemical Physics Letters* 694 (2018) 23-28.
85. Y. Woo, B.-S. Kim, J.-W. Lee, J. Park, M. Cha, S. Takeya, J. Im, Y. Lee, T.-I. Jeon, H. Bae, H. Lee*, S. S. Han, B. C. Yeo, D. Kim, and J.-H. Yoon*, “Enhanced Hydrogen-Storage Capacity and Structural Stability of an Organic Clathrate Structure with Fullerene (C₆₀) Guests and Lithium Doping”, *Chemistry of Materials* 30 (2018) 3028-3039.
86. 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.
87. H. W. Lee, H. Jung, B. C. Yeo, D. Kim, and S. S. Han*, “Atomistic Sodiation Mechanism of Phosphorene-

- Graphene Heterostructure for Sodium-Ion Batteries Determined by First-Principles Calculations”, *Journal of Physical Chemistry C* 122 (2018) 20653-20660.
88. S. Quon,[†] D. Y. Jo,[†] G.-H. Han, S. S. Han, M.-g. Seo,* and K.-Y. Lee,* “Role of Pt Atoms on Pd(111) Surface in the Direct Synthesis of Hydrogen Peroxide: Nano-catalytic Experiments and DFT Calculations”, *Journal of Catalysis* 368 (2018) 237-247.
 89. I. Kim,[†] M.-g. Seo,[†] C. Choi,[†] J. S. Kim, E. Jung, J.-C. Lee, S. S. Han, J.-P. Ahn,* Y. Jung,* K.-Y. Lee,* and T. Yu,* “Studies on Catalytic Activity of Hydrogen Peroxide Generation According to Au Shell Thickness of Pd/Au Nanocubes” *ACS Applied Materials & Interfaces* 10 (2018) 38109-38116 ([†]Equally contributed).
 90. K. Y. Cho,[†] J. Y. Seo,[†] H.-J. Kim, S. J. Pai, X. H. Do, H. G. Yoon, S. S. Hwang, S. S. Han, and K.-Y. Baek,* “Facile Control of Defect Site Density and Particle Size of UiO-66 for Enhanced Hydrolysis Rates: Insights into Feasibility of Zr(IV)-based Metal-Organic Framework (MOF) Catalysts”, *Applied Catalysis B: Environmental* 245 (2019) 635-647 ([†]Equally contributed).
 91. B. C. Yeo, D. Kim, C. Kim, and S. S. Han*, “Pattern Learning Electronic Density of States”, *Scientific Reports*, 9 (2019) 5879(1)-(10).
 92. 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 H₂O₂ Synthesis”, *ACS Catalysis*, 9 (2019) 8702-8711 ([†]Equally contributed).
 93. S. J. Pai, H. W. Lee, and S. S. Han*, “Improved Description of a Coordinate Bond in the ReaxFF Reactive Force Field”, *The Journal of Physical Chemistry Letters*, 10 (2019) 7293-7299.
 94. B. C. Yeo,[†] J. Kong,[†] D. Kim, W. A. Goddard III, H. S. Park,* and S. S. Han*, “Electronic Structural Origin of the Catalytic Activity Trend of Transition Metals for Electrochemical Nitrogen Reduction”, *The Journal of Physical Chemistry C*, 123 (2019) 31026-31031 ([†]Equally contributed).
 95. Y.-H. Cho, G.-H. Han, S. S. Han, M.-g. Seo,* and K.-Y. Lee,* “Effects of Varying Amounts of Na on Pd/TiO₂ for the Direct Synthesis of H₂O₂: Identification of the Pd Dispersion and Catalytic Activity Enhancement by Changing the Surface Electronic States”, *Molecular Catalysis*, 484 (2020) 110732(1)-(8).
 96. M. Kim,[†] B. C. Yeo,[†] Y. Park, H. M. Lee, S. S. Han*, and D. Kim,* “Artificial Intelligence to Accelerate the Discovery of N₂ Electroreduction Catalysts”, *Chemistry of Materials*, 32 (2020) 709-720 ([†]Equally contributed).
 97. D. L. T. Nguyen, C. W. Lee, J. Na, M.-C. Kim, N. D. K. Tu, S. Y. Lee, Y. J. Sa, D. H. Won, H.-S. Oh, H. Kim, B. K. Min, S. S. Han, U. Lee,* and Y. J. Hwang,* “Mass Transport Control by Surface Graphene Oxide for Selective CO Production from Electrochemical CO₂ Reduction”, *ACS Catalysis*, 10 (2020) 3222-3231 ([†]Equally contributed).
 98. 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 (2020) 10577-10584 ([†]Equally contributed).
 99. L. C. O. Tiong,[†] J. Kim,[†] S. S. Han*, and D. Kim,* “Identification of Crystal Symmetry from Noisy Diffraction Patterns by A Shape Analysis and Deep Learning”, *npj Computational Materials*, 6 (2020) 196(1)-(11) ([†]Equally contributed).
 100. 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,* and S.

- S. Han,* “Solid-Solution Alloying of Immiscible Pt and Au Boosts Catalytic Performance for Direct H₂O₂ Synthesis”, *Acta Materialia*, 205 (2021) 116563(1)-(7) (†Equally contributed).
101. M. J. Banisalman, H. W. Lee, H. Koh, and S. S. Han,* “Atomistic Insights into H₂O₂ Direct Synthesis of Ni-Pt Nanoparticle Catalysts under Water Solvents by Reactive Molecular Dynamics Simulations”, *ACS Applied Materials Interfaces*, 13 (2021) 17577-17585.
102. M.-C. Kim and S. S. Han,* “Electrochemically Modeling a Nonelectrochemical System: Hydrogen Peroxide Direct Synthesis on Palladium Catalysts”, *Journal of Physical Chemistry Letters*, 12 (2021) 4490-4495.
103. M.-C. Kim,† G.-H. Han,† X. Xiao,† J. Song,† J. Hong, E. Jung, H.-K. Kim, J.-P. Ahn,* S. S. Han,* K.-Y. Lee,* and T. Yu,* “Anisotropic Growth of Pt on Pd Nanocubes Promotes Direct Synthesis of Hydrogen Peroxide”, *Applied Surface Science*, 562 (2021) 150031 (†Equally contributed).
104. K. Bang, B. C. Yeo, D. Kim, S. S. Han,* and H. M. Lee,* “Accelerated Mapping of Electronic Density of States Patterns of Metallic Nanoparticles Via Machine-Learning”, *Scientific Reports*, 11 (2021) 11604 (arXiv:2007.10646).
105. 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 (2021) 137 (†Equally contributed). (arXiv:2009.08048)
106. J. Kim,† L. C. O. Tiong,† D. Kim,* and S. S. Han,* “Deep Learning-Based Prediction of Material Properties Using Chemical Compositions and Diffraction Patterns as Experimentally Accessible Inputs”, *Journal of Physical Chemistry Letters*, 12 (2021) 8376-8383 (†Equally contributed).
107. H. W. Lee,† E. Jung,† G.-H. Han, M.-C. Kim, D. Kim, K.-Y. Lee,* S. S. Han,* and T. Yu,* “Three-in-One Strategy to Improve Both Catalytic Activity and Selectivity: Nonconcentric Pd-Au Nanoparticles”, *Journal of Physical Chemistry Letters*, 12 (2021) 11098-11105 (†Equally contributed).
108. 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 (2022) 1090-1097.
109. H. W. Lee,† G.-U. Jeong,† M.-C. Kim, D. Kim,* S. Kim,* and S. S. Han,* “Atomistic Origin of Mechanochemical NH₃ Synthesis on Fe Catalysts”, *Int. J. Hydrogen Energy*, 48 (2023) 2931-3941.
110. M.-C. Kim,† J. Chung,† T.-Y. An,† J. Lee, M.-K. Han, S. S. Han,* U. Sim,* and T. Yu,* “Paradox of Thiourea: A False-Positive and Promoter for Electrochemical Nitrogen Reduction on Nickel Sulfide Catalysts”, *Applied Catalysis B: Environment*, 328 (2023) 122485 (†Equally contributed).
111. A. Byeon,† J. W. Choi,† H. W. Lee,† W. C. Yun, W. Zhang, C.-K. Hwang, S. Y. Lee, S. S. Han,* J. M. Kim,* and J. W. Lee,* “CO₂-Derived Edge-Boron-Doped Hierarchical Porous Carbon Catalysts for Highly Effective Electrochemical H₂O₂ Production”, *Applied Catalysis B: Environment*, 329 (2023) 122557 (†Equally contributed).
112. W. Zhang,† J. W. Choi,† S. Kim,† T. T. Le, C.-K. Hwang, S. Y. Paek, K. H. Chae, S. Y. Lee, S. H. Kim, H. Song, J. Kim, J. Oh, S. S. Han,* and J. M. Kim,* “Penta Nitrogen Coordinated Cobalt Single Atom Catalysts with Oxygenated Carbon Black for Enhanced Electrochemical H₂O₂ Synthesis and the Electro-Fenton Process”, *Applied Catalysis B: Environment*, 331 (2023) 122712 (†Equally contributed).
113. K. Bang, D. Hong, Y. Park, D. Kim,* S. S. Han,* and H. M. Lee,* “Machine Learning-Enabled Exploration of

- the Electrochemical Stability of Real-Scale Metallic Nanoparticles”, *Nature Communications*, 14 (2023) 3004.
114. C.-H. Chan, S. Y. Lee, and S. S. Han*, “Origin of Enhanced Toluene Hydrogenation by Pt-Ru Catalysts for an Efficient Liquid Organic Hydrogen Carrier”, *International Journal of Hydrogen Energy*, 48 (2023) 33590-33598.
115. J. Choi,[†] K. Bang,[†] S. Jang, J. W. Choi, J. Ordonez, D. Buttler, A. Hiszpanski, T. Yong-Jin Han, S. S. Sohn, B. Lee, K.-R. Lee, S. S. Han*, and D. Kim*, “Deep Learning of CO₂ Conversion Literature Reveals Research Trends and Directions”, *Journal of Materials Chemistry A*, 11 (2023) 17628 ([†]Equally contributed).
116. Y. Park,[†] C.-K. Hwang,[†] K. Bang, D. hong, H. Nam, S. Kwon, B. C. Yeo, D. Go, J. An, B.-K. Ju, S. H. Kim, J. Y. Byun, S. Y. Lee, M. Kim,* D. Kim,* S. S. Han*, H. M. Lee,* “Machine Learning Filters Out Efficient Electrocatalysts in the Massive Ternary Alloy Space for Fuel Cells”, *Applied Catalysis B: Environmental*, 339 (2023) 123128 ([†]Equally contributed).
117. S. Kim,[†] M.-C. Kim,[†] B. C. Yeo, S. S. Han*, “High-Throughput Design of Bimetallic Core-Shell Catalysts for Electrochemical Nitrogen Reduction Reaction”, *Journal of Materials Chemistry A*, 11 (2024) 24686-24697 ([†]Equally contributed).
118. S. Kim,[†] Y. Lee,[†] K. Kim, B. C. Wood,* S. S. Han*, S. Yu,* “Fluorine-Substituted Lithium Chloride Solid Electrolytes for High-Voltage All-Solid-State Lithium-Ion Batteries”, *ACS Energy Letters*, 9 (2024) 38-47 ([†]Equally contributed).
119. S. Venkateswalu,[†] S. Kim,[†] M. Balamurugan, Y. Son, S.-I. Choi, M. Yoon, K. T. Nam, S. S. Han*, M. J. Kim,* “Boron Nitride Nanotubes Supported Icosahedral Pd Nanoparticles: Enabling Ultrahigh Current Density-Superior Hydrogen Evolution Activity and Theoretical Insights”, *Applied Catalysis B: Environmental*, 345 (2024) 123609 ([†]Equally contributed).
120. L. C. O. Tiong,[†] H. J. Yoo,[†] N. Kim, C. S. Hong, K.-Y. Lee,* S. S. Han*, D. Kim,* “Machine vision-based detections of transparent chemical vessels toward the safe automation of materials synthesis”, *npj Computational Materials*, Accepted (2024) ([†]Equally contributed).
121. K. Bang,[†] J. Kim,[†] D. Hong,[†] D. Kim,* S. S. Han*, “Inverse Design for Materials Discovery from Multidimensional Electronic Density of States”, *Journal of Materials Chemistry A*, Accepted (2024) ([†]Equally contributed).