Sang Soo Han

List of Publications by Year
in descending order

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70	4,757	136950	95266
papers	citations	32 h-index	68 g-index

70	70	70	6210
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Origin of Enhanced Ammonia Synthesis on Ruâ€“Co Catalysts Unraveled by Density Functional Theory. ACS Catalysis, 2022, 12, 1090-1097.	11.2	25
2	Solid-solution alloying of immiscible Pt and Au boosts catalytic performance for H2O2 direct synthesis. Acta Materialia, 2021, 205, 116563.	7.9	10
3	Atomistic Insights into H₂O₂ Direct Synthesis of Niâ€“Pt Nanoparticle Catalysts under Water Solvents by Reactive Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2021, 13, 17577-17585.	8.0	7
4	Electrochemically Modeling a Nonelectrochemical System: Hydrogen Peroxide Direct Synthesis on Palladium Catalysts. Journal of Physical Chemistry Letters, 2021, 12, 4490-4495.	4.6	4
5	Accelerated mapping of electronic density of states patterns of metallic nanoparticles via machine-learning. Scientific Reports, 2021, 11, 11604.	3.3	11
6	High-throughput computational-experimental screening protocol for the discovery of bimetallic catalysts. Npj Computational Materials, 2021, 7, .	8.7	20
7	Deep Learning-Based Prediction of Material Properties Using Chemical Compositions and Diffraction Patterns as Experimentally Accessible Inputs. Journal of Physical Chemistry Letters, 2021, 12, 8376-8383.	4.6	5
8	Anisotropic growth of Pt on Pd nanocube promotes direct synthesis of hydrogen peroxide. Applied Surface Science, 2021, 562, 150031.	6.1	16
9	Three-in-One Strategy to Improve Both Catalytic Activity and Selectivity: Nonconcentric Pdâ€“Au Nanoparticles. Journal of Physical Chemistry Letters, 2021, 12, 11098-11105.	4.6	5
10	Artificial Intelligence to Accelerate the Discovery of N₂ Electroreduction Catalysts. Chemistry of Materials, 2020, 32, 709-720.	6.7	59
11	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, 2020, 484, 110732.	2.0	2
12	Hydrogen Bonding-Mediated Enhancement of Bioinspired Electrochemical Nitrogen Reduction on Cu_{2â€“x}S Catalysts. ACS Catalysis, 2020, 10, 10577-10584.	11.2	43
13	Mass Transport Control by Surface Graphene Oxide for Selective CO Production from Electrochemical CO₂ Reduction. ACS Catalysis, 2020, 10, 3222-3231.	11.2	57
14	Identification of crystal symmetry from noisy diffraction patterns by a shape analysis and deep learning. Npj Computational Materials, 2020, 6, .	8.7	23
15	Unlocking the Potential of Nanoparticles Composed of Immiscible Elements for Direct H2O2 Synthesis. ACS Catalysis, 2019, 9, 8702-8711.	11.2	32
16	Improved Description of a Coordinate Bond in the ReaxFF Reactive Force Field. Journal of Physical Chemistry Letters, 2019, 10, 7293-7299.	4.6	7
17	Pattern Learning Electronic Density of States. Scientific Reports, 2019, 9, 5879.	3.3	38
18	Electronic Structural Origin of the Catalytic Activity Trend of Transition Metals for Electrochemical Nitrogen Reduction. Journal of Physical Chemistry C, 2019, 123, 31026-31031.	3.1	16

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19	Enhanced Hydrogen-Storage Capacity and Structural Stability of an Organic Clathrate Structure with Fullerene (C₆₀) Guests and Lithium Doping. Chemistry of Materials, 2018, 30, 3028-3039.	6.7	22
20	Role of Pt atoms on Pd(1â€¯1â€¯1) surface in the direct synthesis of hydrogen peroxide: Nano-catalytic experiments and DFT calculations. Journal of Catalysis, 2018, 368, 237-247.	6.2	38
21	Studies on Catalytic Activity of Hydrogen Peroxide Generation according to Au Shell Thickness of Pd/Au Nanocubes. ACS Applied Materials & Interfaces, 2018, 10, 38109-38116.	8.0	32
22	Activity, Selectivity, and Durability of Ruthenium Nanoparticle Catalysts for Ammonia Synthesis by Reactive Molecular Dynamics Simulation: The Size Effect. ACS Applied Materials & Interfaces, 2018, 10, 26188-26194.	8.0	27
23	Atomistic Sodiation Mechanism of a Phosphorene/Graphene Heterostructure for Sodium-Ion Batteries Determined by First-Principles Calculations. Journal of Physical Chemistry C, 2018, 122, 20653-20660.	3.1	35
24	Highly dispersed Pd catalysts prepared by a sonochemical method for the direct synthesis of hydrogen peroxide. Molecular Catalysis, 2017, 429, 43-50.	2.0	23
25	Dissimilar anisotropy of electron versus hole bulk transport in anatase <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></m : Implications for photocatalysis. Physical Review B, 2017, 95, .	3.2	28
26	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, 2017, 8, 2812-2818.	4.6	51
27	ReaxFF Molecular Dynamics Simulations of Water Stability of Interpenetrated Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2017, 121, 7312-7318.	3.1	15
28	Direct Synthesis of Hydrogen Peroxide from Hydrogen and Oxygen over Mesoporous Silica-Shell-Coated, Palladium-Nanocrystal-Grafted SiO₂ Nanobeads. ACS Catalysis, 2017, 7, 3039-3048.	11.2	60
29	Atomistic Simulation Protocol for Improved Design of Siâ€“Oâ€“C Hybrid Nanostructures as Li-Ion Battery Anodes: ReaxFF Reactive Force Field. Journal of Physical Chemistry C, 2017, 121, 23268-23275.	3.1	14
30	Î²-CuGaO₂ as a Strong Candidate Material for Efficient Ferroelectric Photovoltaics. Chemistry of Materials, 2017, 29, 7596-7603.	6.7	28
31	S _E 2 reaction in noncarbon system: Metal-halide catalysis for dehydrogenation of ammonia borane. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 13625-13630.	7.1	4
32	Reaction Mechanism of Area-Selective Atomic Layer Deposition for Al₂O₃ Nanopatterns. ACS Applied Materials & Interfaces, 2017, 9, 41607-41617.	8.0	73
33	Direct Synthesis of Hydrogen Peroxide from Hydrogen and Oxygen Using Tailored Pd Nanocatalysts: A Review of Recent Findings. Catalysis Surveys From Asia, 2017, 21, 1-12.	2.6	58
34	A comparative first-principles study of the lithiation, sodiation, and magnesiation of black phosphorus for Li-, Na-, and Mg-ion batteries. Physical Chemistry Chemical Physics, 2016, 18, 21391-21397.	2.8	73
35	Atomistics of the lithiation of oxidized silicon (SiO_x) nanowires in reactive molecular dynamics simulations. Physical Chemistry Chemical Physics, 2016, 18, 32078-32086.	2.8	41
36	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, 2016, 22, 7444-7451.	3.3	30

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37	Thermostable Artificial Solid-Electrolyte Interface Layer Covalently Linked to Graphite for Lithium Ion Battery: Molecular Dynamics Simulations. Journal of the Electrochemical Society, 2016, 163, A917-A922.	2.9	16
38	Development of the ReaxFF_{CBN} reactive force field for the improved design of liquid CBN hydrogen storage materials. Physical Chemistry Chemical Physics, 2016, 18, 1818-1827.	2.8	27
39	Atomistic Observation of the Lithiation and Delithiation Behaviors of Silicon Nanowires Using Reactive Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2015, 119, 3447-3455.	3.1	56
40	Unraveling the Atomistic Sodiation Mechanism of Black Phosphorus for Sodium Ion Batteries by First-Principles Calculations. Journal of Physical Chemistry C, 2015, 119, 15041-15046.	3.1	135
41	Exceptional CO₂ working capacity in a heterodiamine-grafted metalâ€“organic framework. Chemical Science, 2015, 6, 3697-3705.	7.4	127
42	Diamine-functionalized metalâ€“organic framework: exceptionally high CO₂capacities from ambient air and flue gas, ultrafast CO₂uptake rate, and adsorption mechanism. Energy and Environmental Science, 2014, 7, 744-751.	30.8	260
43	Reply to the â€˜Comment on â€œVolume shrinkage of a metalâ€“organic framework host induced by the dispersive attraction of guest gas moleculesâ€â€™ by F.-X. Coudert, A. H. Fuchs, and A. V. Neimark, Phys. Chem. Chem. Phys.. Physical Chemistry Chemical Physics, 2014, 16, 4396.	2.8	0
44	First-Principles Design of Hydrogen Dissociation Catalysts Based on Isoelectronic Metal Solid Solutions. Journal of Physical Chemistry Letters, 2014, 5, 1819-1824.	4.6	26
45	Lithiumâ€Functionalized Metalâ€“Organic Frameworks that Show >10 wtâ€‰% H 2 Uptake at Ambient Temperature. ChemPhysChem, 2013, 14, 2698-2703.	2.1	6
46	Volume shrinkage of a metalâ€“organic framework host induced by the dispersive attraction of guest gas molecules. Physical Chemistry Chemical Physics, 2013, 15, 18822.	2.8	23
47	Interpenetration of Metal Organic Frameworks for Carbon Dioxide Capture and Hydrogen Purification: Good or Bad?. Journal of Physical Chemistry C, 2013, 117, 71-77.	3.1	38
48	Tuning Metalâ€“Organic Frameworks with Open-Metal Sites and Its Origin for Enhancing CO₂ Affinity by Metal Substitution. Journal of Physical Chemistry Letters, 2012, 3, 826-829.	4.6	116
49	Improved H₂ Storage in Zeolitic Imidazolate Frameworks Using Li⁺, Na⁺, and K⁺ Dopants, with an Emphasis on Delivery H₂ Uptake. Journal of Physical Chemistry C, 2011, 115, 3507-3512.	3.1	37
50	Adsorption Mechanism and Uptake of Methane in Covalent Organic Frameworks: Theory and Experiment. Journal of Physical Chemistry A, 2010, 114, 10824-10833.	2.5	177
51	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, 2010, 114, 3156-3160.	3.1	32
52	Molecular dynamics simulations of stability of metalâ€“organic frameworks against H2O using the ReaxFF reactive force field. Chemical Communications, 2010, 46, 5713.	4.1	121
53	Zeolitic Imidazolate Frameworks as H2 Adsorbents: Ab Initio Based Grand Canonical Monte Carlo Simulation. Journal of Physical Chemistry C, 2010, 114, 12039-12047.	3.1	57
54	Recent advances on simulation and theory of hydrogen storage in metalâ€“organic frameworks and covalent organic frameworks. Chemical Society Reviews, 2009, 38, 1460.	38.1	535

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55	A hydrogen storage nanotank: lithium-organic pillared graphite. Chemical Communications, 2009, , 5427.	4.1	16
56	Covalent Organic Frameworks as Exceptional Hydrogen Storage Materials. Journal of the American Chemical Society, 2008, 130, 11580-11581.	13.7	746
57	High H2 Storage of Hexagonal Metalâ^'Organic Frameworks from First-Principles-Based Grand Canonical Monte Carlo Simulations. Journal of Physical Chemistry C, 2008, 112, 13431-13436.	3.1	71
58	Metalâ^'Organic Frameworks Provide Large Negative Thermal Expansion Behavior. Journal of Physical Chemistry C, 2007, 111, 15185-15191.	3.1	170
59	Lithium-Doped Metal-Organic Frameworks for Reversible H₂ Storage at Ambient Temperature. Journal of the American Chemical Society, 2007, 129, 8422-8423.	13.7	418
60	Improved Designs of Metalâ€"Organic Frameworks for Hydrogen Storage. Angewandte Chemie - International Edition, 2007, 46, 6289-6292.	13.8	212
61	Theoretical study on interaction of hydrogen with single-walled boron nitride nanotubes. II. Collision, storage, and adsorption. Journal of Chemical Physics, 2005, 123, 114704.	3.0	44
62	Nanopores of carbon nanotubes as practical hydrogen storage media. Applied Physics Letters, 2005, 87, 213113.	3.3	31
63	Atmospheric-pressure plasma treatment to modify hydrogen storage properties of multiwalled carbon nanotubes. Applied Physics Letters, 2005, 86, 263105.	3.3	17
64	Liquefaction of H2 molecules upon exterior surfaces of carbon nanotube bundles. Applied Physics Letters, 2005, 86, 203108.	3.3	30
65	Optimization and Application of Lithium Parameters for the Reactive Force Field, ReaxFF. Journal of Physical Chemistry A, 2005, 109, 4575-4582.	2.5	92
66	The theoretical study on interaction of hydrogen with single-walled boron nitride nanotubes. I. The reactive force field ReaxFFHBN development. Journal of Chemical Physics, 2005, 123, 114703.	3.0	54
67	Nanomechanical Behavior of β-SiC Nanowire in Tension: Molecular Dynamics Simulations. Materials Transactions, 2004, 45, 1442-1449.	1.2	33
68	Study on Cap Closure Mechanism of Single-Walled Carbon Nanotubes by Molecular Dynamics. Materials Transactions, 2004, 45, 1437-1441.	1.2	0
69	Molecular dynamics simulation of zigzag single-walled carbon nanotube closing mechanisms. Metals and Materials International, 2003, 9, 99-105.	3.4	4
70	Three-dimensional monte-carlo simulation of grain growth in Pt-Co thin film. Journal of Electronic Materials, 2002, 31, 965-971.	2.2	3