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	Covalent Organic Frameworks as Exceptional Hydrogen Storage Materials. Journal of the American Chemical Society, 2008, 130, 11580-11581.	13.7	746
2	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
3	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
4	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
5	Improved Designs of Metalâ€“Organic Frameworks for Hydrogen Storage. Angewandte Chemie - International Edition, 2007, 46, 6289-6292.	13.8	212
6	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
7	Metalâ^'Organic Frameworks Provide Large Negative Thermal Expansion Behavior. Journal of Physical Chemistry C, 2007, 111, 15185-15191.	3.1	170
8	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
9	Exceptional CO₂ working capacity in a heterodiamine-grafted metalâ€“organic framework. Chemical Science, 2015, 6, 3697-3705.	7.4	127
10	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
11	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
12	Optimization and Application of Lithium Parameters for the Reactive Force Field, ReaxFF. Journal of Physical Chemistry A, 2005, 109, 4575-4582.	2.5	92
13	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
14	Reaction Mechanism of Area-Selective Atomic Layer Deposition for Al₂O₃ Nanopatterns. ACS Applied Materials & Interfaces, 2017, 9, 41607-41617.	8.0	73
15	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
16	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
17	Artificial Intelligence to Accelerate the Discovery of N₂ Electroreduction Catalysts. Chemistry of Materials, 2020, 32, 709-720.	6.7	59
18	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

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19	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
20	Mass Transport Control by Surface Graphene Oxide for Selective CO Production from Electrochemical CO₂ Reduction. ACS Catalysis, 2020, 10, 3222-3231.	11.2	57
21	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
22	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
23	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
24	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
25	Hydrogen Bonding-Mediated Enhancement of Bioinspired Electrochemical Nitrogen Reduction on Cu_{2â€“x}S Catalysts. ACS Catalysis, 2020, 10, 10577-10584.	11.2	43
26	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
27	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
28	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
29	Pattern Learning Electronic Density of States. Scientific Reports, 2019, 9, 5879.	3.3	38
30	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
31	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
32	Nanomechanical Behavior of β-SiC Nanowire in Tension: Molecular Dynamics Simulations. Materials Transactions, 2004, 45, 1442-1449.	1.2	33
33	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
34	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
35	Unlocking the Potential of Nanoparticles Composed of Immiscible Elements for Direct H2O2 Synthesis. ACS Catalysis, 2019, 9, 8702-8711.	11.2	32
36	Nanopores of carbon nanotubes as practical hydrogen storage media. Applied Physics Letters, 2005, 87, 213113.	3.3	31

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37	Liquefaction of H2 molecules upon exterior surfaces of carbon nanotube bundles. Applied Physics Letters, 2005, 86, 203108.	3.3	30
38	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
39	Î²-CuGaO₂ as a Strong Candidate Material for Efficient Ferroelectric Photovoltaics. Chemistry of Materials, 2017, 29, 7596-7603.	6.7	28
40	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
41	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
42	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
43	Origin of Enhanced Ammonia Synthesis on Ruâ€“Co Catalysts Unraveled by Density Functional Theory. ACS Catalysis, 2022, 12, 1090-1097.	11.2	25
44	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
45	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
46	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></mml: : Implications for photocatalysis. Physical Review B, 2017, 95, .	3.2	23
47	Identification of crystal symmetry from noisy diffraction patterns by a shape analysis and deep learning. Npj Computational Materials, 2020, 6, .	8.7	23
48	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
49	High-throughput computational-experimental screening protocol for the discovery of bimetallic catalysts. Npj Computational Materials, 2021, 7, .	8.7	20
50	Atmospheric-pressure plasma treatment to modify hydrogen storage properties of multiwalled carbon nanotubes. Applied Physics Letters, 2005, 86, 263105.	3.3	17
51	A hydrogen storage nanotank: lithium-organic pillared graphite. Chemical Communications, 2009, , 5427.	4.1	16
52	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
53	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
54	Anisotropic growth of Pt on Pd nanocube promotes direct synthesis of hydrogen peroxide. Applied Surface Science, 2021, 562, 150031.	6.1	16

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55	ReaxFF Molecular Dynamics Simulations of Water Stability of Interpenetrated Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2017, 121, 7312-7318.	3.1	15
56	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
57	Accelerated mapping of electronic density of states patterns of metallic nanoparticles via machine-learning. Scientific Reports, 2021, 11, 11604.	3.3	11
58	Solid-solution alloying of immiscible Pt and Au boosts catalytic performance for H2O2 direct synthesis. Acta Materialia, 2021, 205, 116563.	7.9	10
59	Improved Description of a Coordinate Bond in the ReaxFF Reactive Force Field. Journal of Physical Chemistry Letters, 2019, 10, 7293-7299.	4.6	7
60	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
61	Lithiumâ€Functionalized Metalâ€“Organic Frameworks that Show >10 wtâ€‰% H 2 Uptake at Ambient Temperature. ChemPhysChem, 2013, 14, 2698-2703.	2.1	6
62	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
63	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
64	Molecular dynamics simulation of zigzag single-walled carbon nanotube closing mechanisms. Metals and Materials International, 2003, 9, 99-105.	3.4	4
65	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
66	Electrochemically Modeling a Nonelectrochemical System: Hydrogen Peroxide Direct Synthesis on Palladium Catalysts. Journal of Physical Chemistry Letters, 2021, 12, 4490-4495.	4.6	4
67	Three-dimensional monte-carlo simulation of grain growth in Pt-Co thin film. Journal of Electronic Materials, 2002, 31, 965-971.	2.2	3
68	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
69	Study on Cap Closure Mechanism of Single-Walled Carbon Nanotubes by Molecular Dynamics. Materials Transactions, 2004, 45, 1437-1441.	1.2	0
70	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