

Lei Sun

List of Publications by Year in descending order

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74
papers

4,249
citations

218677

26
h-index

110387

64
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76
all docs

76
docs citations

76
times ranked

6203
citing authors

#	ARTICLE	IF	CITATIONS
1	Selectively nitrogen-doped carbon materials as superior metal-free catalysts for oxygen reduction. Nature Communications, 2018, 9, 3376.	12.8	436
2	Coupling Subnanometric Copper Clusters with Quasi-Amorphous Cobalt Sulfide Yields Efficient and Robust Electrocatalysts for Water Splitting Reaction. Advanced Materials, 2017, 29, 1606200.	21.0	350
3	Efficient electrocatalysis of overall water splitting by ultrasmall NiCo ₃ S ₄ coupled Ni ₃ S ₂ nanosheet arrays. Nano Energy, 2017, 35, 161-170.	16.0	339
4	Lead-Free Silver-Bismuth Halide Double Perovskite Nanocrystals. Angewandte Chemie - International Edition, 2018, 57, 5359-5363.	13.8	281
5	In Situ Generation of Bifunctional, Efficient Fe-Based Catalysts from Mackinawite Iron Sulfide for Water Splitting. Chem, 2018, 4, 1139-1152.	11.7	271
6	Conductive Microporous Covalent Triazine-Based Framework for High-Performance Electrochemical Capacitive Energy Storage. Angewandte Chemie - International Edition, 2018, 57, 7992-7996.	13.8	193
7	Colloidal Synthesis and Optical Properties of All-Inorganic Low-Dimensional Cesium Copper Halide Nanocrystals. Angewandte Chemie - International Edition, 2019, 58, 16087-16091.	13.8	192
8	Quantitative prediction of charge mobilities of π -stacked systems by first-principles simulation. Nature Protocols, 2015, 10, 632-642.	12.0	187
9	Constructing Connected Paths between UiO-66 and PIM-1 to Improve Membrane CO ₂ Separation with Crystal-Like Gas Selectivity. Advanced Materials, 2019, 31, e1806853.	21.0	187
10	In situ photodeposition of platinum clusters on a covalent organic framework for photocatalytic hydrogen production. Nature Communications, 2022, 13, 1355.	12.8	140
11	Lead-Free Silver-Bismuth Halide Double Perovskite Nanocrystals. Angewandte Chemie, 2018, 130, 5457-5461.	2.0	132
12	Revealing Activity Trends of Metal Diborides Toward pH-Universal Hydrogen Evolution Electrocatalysts with Pt-Like Activity. Advanced Energy Materials, 2019, 9, 1803369.	19.5	111
13	Theoretical Investigation of CO ₂ Adsorption and Dissociation on Low Index Surfaces of Transition Metals. Journal of Physical Chemistry C, 2018, 122, 8306-8314.	3.1	104
14	First-Principles Screening of All-Inorganic Lead-Free ABX ₃ Perovskites. Journal of Physical Chemistry C, 2018, 122, 7670-7675.	3.1	98
15	Colloidal Synthesis and Optical Properties of All-Inorganic Low-Dimensional Cesium Copper Halide Nanocrystals. Angewandte Chemie, 2019, 131, 16233-16237.	2.0	78
16	Lead-free and stable antimony-silver-halide double perovskite (CH ₃ NH ₃) ₂ AgSbI ₆ . RSC Advances, 2017, 7, 35175-35180.	3.6	75
17	Revealing the Relationship between Energy Level and Gas Sensing Performance in Heteroatom-Doped Semiconducting Nanostructures. ACS Applied Materials & Interfaces, 2018, 10, 29795-29804.	8.0	74
18	Enhanced carbon dioxide conversion at ambient conditions via a pore enrichment effect. Nature Communications, 2020, 11, 4481.	12.8	74

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19	Conductive Microporous Covalent Triazine-Based Framework for High-Performance Electrochemical Capacitive Energy Storage. <i>Angewandte Chemie</i> , 2018, 130, 8124-8128.	2.0	67
20	A Schiff base-modified silver catalyst for efficient fixation of CO ₂ as carboxylic acid at ambient pressure. <i>Green Chemistry</i> , 2017, 19, 2080-2085.	9.0	65
21	Well-Tuned Surface Oxygen Chemistry of Cation Off-Stoichiometric Spinel Oxides for Highly Selective and Sensitive Formaldehyde Detection. <i>Chemistry of Materials</i> , 2018, 30, 2018-2027.	6.7	64
22	On the mechanism of H ₂ activation over single-atom catalyst: An understanding of Pt ₁ /WO ₃ in the hydrogenolysis reaction. <i>Chinese Journal of Catalysis</i> , 2020, 41, 524-532.	14.0	50
23	Chemical fixation of carbon dioxide catalyzed <i>via</i> covalent triazine frameworks as metal free heterogeneous catalysts without a cocatalyst. <i>Journal of Materials Chemistry A</i> , 2019, 7, 26071-26076.	10.3	39
24	Niobium-Doped (001)-Dominated Anatase TiO ₂ Nanosheets as Photoelectrode for Efficient Dye-Sensitized Solar Cells. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 9576-9583.	8.0	36
25	In Silico Design of Covalent Organic Framework-Based Electrocatalysts. <i>Jacs Au</i> , 2021, 1, 1497-1505.	7.9	28
26	A zeolite-like aluminophosphate membrane with molecular-sieving property for water desalination. <i>Chemical Science</i> , 2018, 9, 2533-2539.	7.4	27
27	Accurate van der Waals force field for gas adsorption in porous materials. <i>Journal of Computational Chemistry</i> , 2017, 38, 1991-1999.	3.3	26
28	Pt/ZSM-22 with Partially Filled Micropore Channels as Excellent Shape-Selective Hydroisomerization Catalyst. <i>ChemCatChem</i> , 2019, 11, 1431-1436.	3.7	26
29	First-Principles Screening of Lead-Free Methylammonium Metal Iodine Perovskites for Photovoltaic Application. <i>Journal of Physical Chemistry C</i> , 2017, 121, 24359-24364.	3.1	25
30	Unblocked intramolecular charge transfer for enhanced CO ₂ photoreduction enabled by an imidazolium-based ionic conjugated microporous polymer. <i>Applied Catalysis B: Environmental</i> , 2022, 300, 120719.	20.2	25
31	Enantioselective Synthesis of 3,4-Dihydropyrimidin-2(1 <i>H</i>)-ones through Organocatalytic Transfer Hydrogenation of 2-Hydroxypyrimidines. <i>Journal of Organic Chemistry</i> , 2019, 84, 4435-4442.	3.2	24
32	Fabrication and evaluation of effective zeolite membranes for water desalination. <i>Desalination</i> , 2021, 504, 114974.	8.2	22
33	Hollow Multi-Shelled V ₂ O ₅ Microstructures Integrating Multiple Synergistic Resonances for Enhanced Semiconductor SERS. <i>Advanced Optical Materials</i> , 2021, 9, 2101866.	7.3	22
34	Iron single-atom catalysts confined in covalent organic frameworks for efficient oxygen evolution reaction. <i>Cell Reports Physical Science</i> , 2022, 3, 100804.	5.6	22
35	Ship emission of nitrous acid (HONO) and its impacts on the marine atmospheric oxidation chemistry. <i>Science of the Total Environment</i> , 2020, 735, 139355.	8.0	21
36	Copper-Catalyzed Alkynylation/Cyclization/Isomerization Cascade for Synthesis of 1,2-Dihydrobenzofuro[3,2- <i>b</i>]pyridines and Benzofuro[3,2- <i>b</i>]pyridines. <i>Journal of Organic Chemistry</i> , 2019, 84, 15498-15507.	3.2	19

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37	Recent developments of first-principles force fields. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1282.	14.6	18
38	Ambient hydrogenation of carbon dioxide into liquid fuel by a heterogeneous synergetic dual single-atom catalyst. Cell Reports Physical Science, 2022, 3, 100705.	5.6	18
39	Diffusion of tungsten clusters on tungsten (110) surface. European Physical Journal B, 2009, 68, 479-485.	1.5	17
40	Enantioselective Carbene Insertion into O-H of Phenols with Chiral Palladium/2,2'-Biimidazole Complexes. Organometallics, 2019, 38, 3902-3905.	2.3	17
41	COOH-MWCNT connected COF and chemical activated CTF as a novel electrochemical sensing platform for simultaneous detection of acetaminophen and p-aminophenol. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 647, 129092.	4.7	17
42	Evaluation of the behavior of clouds in a region of severe acid rain pollution in southern China: species, complexes, and variations. Environmental Science and Pollution Research, 2015, 22, 14280-14290.	5.3	16
43	Gold Cluster-CeO ₂ Nanostructured Hybrid Architectures as Catalysts for Selective Oxidation of Inert Hydrocarbons. Chemistry of Materials, 2018, 30, 8579-8586.	6.7	16
44	Hydrogen and CO ₂ storage in high surface area covalent triazine-based frameworks. Materials Today Energy, 2020, 18, 100506.	4.7	16
45	Salen-Based Conjugated Microporous Polymers for Efficient Oxygen Evolution Reaction. Chemistry - A European Journal, 2020, 26, 7720-7726.	3.3	16
46	A DFT Exploration of Efficient Catalysts Based on Metal-Salen Monomers for the Cycloaddition Reaction of CO ₂ to Propylene Oxide. ChemistrySelect, 2017, 2, 4533-4537.	1.5	15
47	A Diarylethene type dye for highly efficient dye-sensitized solar cells. RSC Advances, 2015, 5, 37574-37580.	10.6	13
48	<i>In silico</i> design of dual-doped nitrogenated graphene (C ₂ N) employed in electrocatalytic reduction of carbon monoxide to ethylene. Journal of Materials Chemistry A, 2022, 10, 4703-4710.	10.3	12
49	Cloud deposition of PAHs at Mount Lushan in southern China. Science of the Total Environment, 2015, 526, 329-337.	8.0	11
50	Methylithium-Doped Naphthyl-Containing Conjugated Microporous Polymer with Enhanced Hydrogen Storage Performance. Chemistry - A European Journal, 2016, 22, 7944-7949.	3.3	11
51	Combination Rules for Morse-Based van der Waals Force Fields. Journal of Physical Chemistry A, 2018, 122, 1672-1677.	2.5	11
52	Synthesis, Structure and Tribological Properties of Stearic Acid Coated (NH ₄) ₃ PMo ₁₂ O ₄₀ Nanoparticles. Tribology Letters, 2004, 17, 311-316.	2.6	10
53	Nitrosophthal reaction-assisted SERS assay for selective determination of 5-hydroxyindole-3-acetic acid in human urine. Analytica Chimica Acta, 2020, 1134, 34-40.	5.4	10
54	Theoretical studies on the catalytic hydrogenation of carbon dioxide by 3d transition metals single-atom catalyst supported on covalent triazine frameworks. Molecular Catalysis, 2021, 508, 111581.	2.0	10

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55	Pollution characteristics of particulate matters emitted from outdoor barbecue cooking in urban Jinan in eastern China. <i>Frontiers of Environmental Science and Engineering</i> , 2018, 12, 1.	6.0	9
56	Combination Rules and Accurate van der Waals Force Field for Gas Uptakes in Porous Materials. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7847-7854.	2.5	8
57	First-Principles Screening of Lead-Free Mixed-Anion Perovskites for Photovoltaics. <i>Journal of Physical Chemistry C</i> , 2020, 124, 1303-1308.	3.1	8
58	AUTOMESH ^{2D/3D} : robust automatic mesh generator for metal forming simulation. <i>Materials Research Innovations</i> , 2011, 15, s482-s486.	2.3	7
59	The Second Excited Triplet ¹ State Facilitates TADF and Triplet ³ Triplet Annihilation Photon Upconversion via a Thermally Activated Reverse Internal Conversion. <i>Advanced Optical Materials</i> , 2022, 10, .	7.3	7
60	Conjugated microporous polymer foams with excellent thermal insulation performance in a humid environment. <i>RSC Advances</i> , 2021, 11, 13957-13963.	3.6	4
61	Achieving ultra-low friction of a ² C:H film grown on 9Cr18Mo steel for industrial application via programmable high power pulse magnetron sputtering. <i>Surface and Interface Analysis</i> , 2022, 54, 81-91.	1.8	4
62	Rational Design of Synergistic Structure Between Single-Atoms and Nanoparticles for CO ₂ Hydrogenation to Formate Under Ambient Conditions. <i>Frontiers in Chemistry</i> , 0, 10, .	3.6	3
63	Tungsten cluster migration on nanoparticles: minimum energy pathway and migration mechanism. <i>European Physical Journal B</i> , 2011, 80, 31-40.	1.5	2
64	Carrier mobility in double-helix DNA and RNA: A quantum chemistry study with Marcus-Hush theory. <i>Journal of Chemical Physics</i> , 2016, 145, 235101.	3.0	2
65	van der Waals Function for Molecular Mechanics. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2102-2107.	2.5	2
66	Digital-intellectual design of microporous organic polymers. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 22835-22853.	2.8	2
67	Computational Screening of Zeolite Catalysts for MTO Reaction. <i>ChemistrySelect</i> , 2017, 2, 10290-10294.	1.5	1
68	Molecular-scale observation of YD ₂ -o-C ₈ self-assembled monolayer on TiO ₂ (1 ¹¹ 1 ⁰). <i>Surface Science</i> , 2017, 665, 103-107.	1.9	1
69	In silico design of new nitrogen-rich melamine-based porous polyamides applied to CO ₂ /N ₂ separation. <i>Chemical Physics Letters</i> , 2021, 771, 138509.	2.6	1
70	Progress and Prospect of Theoretical Simulation of Microporous Materials. <i>Acta Chimica Sinica</i> , 2015, 73, 579.	1.4	1
71	In silico design of metal-free hydrophosphate catalysts for hydrogenation of CO ₂ to formate. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 2901-2908.	2.8	1
72	Tribology Dependence of Annealed a-C:H Films in Dry Air and Methanol Environments. <i>ACS Omega</i> , 2022, 7, 7472-7480.	3.5	1

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73	Reliability analysis of rectification on electromagnetic compatibility test. , 2017, , .		0
74	Theoretical design of Salenâ€metal-based materials for highly selective separation of C2H2/C2H4. Chemical Physics Letters, 2021, 771, 138523.	2.6	0