Daojian Cheng

List of Publications by Year
in descending order

91 papers	4,978 citations	136950 32 h-index	95266 68 g-index
94 all docs	94 docs citations	94 times ranked	6075 citing authors

#	ARTICLE	IF	CITATIONS
1	A universal principle for a rational design of single-atom electrocatalysts. Nature Catalysis, 2018, 1, 339-348.	34.4	1,214
2	Unveiling the high-activity origin of single-atom iron catalysts for oxygen reduction reaction. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 6626-6631.	7.1	500
3	Vertical CoP Nanoarray Wrapped by N,Pâ€Doped Carbon for Hydrogen Evolution Reaction in Both Acidic and Alkaline Conditions. Advanced Energy Materials, 2019, 9, 1803970.	19.5	284
4	Singleâ€Atom Ru Doping Induced Phase Transition of MoS₂ and S Vacancy for Hydrogen Evolution Reaction. Small Methods, 2019, 3, 1900653.	8.6	206
5	CoP nanowires coupled with CoMoP nanosheets as a highly efficient cooperative catalyst for hydrogen evolution reaction. Nano Energy, 2020, 68, 104332.	16.0	202
6	Computational Approaches to the Chemical Conversion of Carbon Dioxide. ChemSusChem, 2013, 6, 944-965.	6.8	144
7	Facile Synthesis of Cu/NiCu Electrocatalysts Integrating Alloy, Coreâ€“Shell, and One-Dimensional Structures for Efficient Methanol Oxidation Reaction. ACS Applied Materials & Interfaces, 2017, 9, 19843-19851.	8.0	114
8	Construction of Defectâ€Rich RhCu Nanotubes with Highly Active Rh₃Cu₁ Alloy Phase for Overall Water Splitting in All pH Values. Advanced Energy Materials, 2020, 10, 1903038.	19.5	102
9	Thermal behavior of core-shell and three-shell layered clusters: Melting ofCu1Au54andCu12Au43. Physical Review B, 2006, 74, .	3.2	82
10	Interface construction of P-Substituted MoS2 as efficient and robust electrocatalyst for alkaline hydrogen evolution reaction. Nano Energy, 2020, 78, 105253.	16.0	80
11	Active Site Identification and Evaluation Criteria of In Situ Grown CoTe and NiTe Nanoarrays for Hydrogen Evolution and Oxygen Evolution Reactions. Small Methods, 2019, 3, 1900113.	8.6	78
12	Design of High-Performance Pd-Based Alloy Nanocatalysts for Direct Synthesis of H₂O₂. ACS Catalysis, 2017, 7, 2164-2170.	11.2	75
13	Construction of Dualâ€Site Atomically Dispersed Electrocatalysts with Ruâ€C₅ Single Atoms and Ruâ€O₄ Nanoclusters for Accelerated Alkali Hydrogen Evolution. Small, 2021, 17, e2101163.	10.0	71
14	Identification of activity trends for CO oxidation on supported transition-metal single-atom catalysts. Catalysis Science and Technology, 2017, 7, 5860-5871.	4.1	69
15	Growth of Highly Active Amorphous RuCu Nanosheets on Cu Nanotubes for the Hydrogen Evolution Reaction in Wide pH Values. Small, 2020, 16, e2000924.	10.0	69
16	Understanding the Mechanism of Photocatalysis Enhancements in the Graphene-like Semiconductor Sheet/TiO2 Composites. Journal of Physical Chemistry C, 2014, 118, 5954-5960.	3.1	65
17	Hydrogen Production via Efficient Formic Acid Decomposition: Engineering the Surface Structure of Pd-Based Alloy Catalysts by Design. ACS Catalysis, 2019, 9, 781-790.	11.2	62
18	Fine Tuning Electronic Structure of Catalysts through Atomic Engineering for Enhanced Hydrogen Evolution. Advanced Energy Materials, 2018, 8, 1800789.	19.5	59

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19	Component-dependent electrocatalytic activity of PdCu bimetallic nanoparticles for hydrogen evolution reaction. Electrochimica Acta, 2017, 246, 572-579.	5.2	58
20	Design of high-performance MoS₂ edge supported single-metal atom bifunctional catalysts for overall water splitting <i>via</i> a simple equation. Nanoscale, 2019, 11, 20228-20237.	5.6	57
21	Low Pt-Content Ternary PtNiCu Nanoparticles with Hollow Interiors and Accessible Surfaces as Enhanced Multifunctional Electrocatalysts. ACS Applied Materials & Interfaces, 2020, 12, 9600-9608.	8.0	54
22	Porous Co2P nanowires as high efficient bifunctional catalysts for 4-nitrophenol reduction and sodium borohydride hydrolysis. Journal of Colloid and Interface Science, 2017, 507, 429-436.	9.4	51
23	Tailoring of Pdâ€“Pt bimetallic clusters with high stability for oxygen reduction reaction. Nanoscale, 2012, 4, 2408.	5.6	47
24	Branch-leaf-shaped CuNi@NiFeCu nanodendrites as highly efficient electrocatalysts for overall water splitting. Applied Catalysis B: Environmental, 2021, 298, 120600.	20.2	47
25	SiH/TiO2 and GeH/TiO2 Heterojunctions: Promising TiO2-based Photocatalysts under Visible Light. Scientific Reports, 2014, 4, 4810.	3.3	43
26	Enhanced photoelectrochemical performance of rutile TiO2 by Sb-N donor-acceptor coincorporation from first principles calculations. Applied Physics Letters, 2011, 99, .	3.3	41
27	Growth of IrCu nanoislands with rich IrCu/Ir interfaces enables highly efficient overall water splitting in non-acidic electrolytes. Chemical Engineering Journal, 2021, 416, 129128.	12.7	41
28	From doubleâ€atom catalysts to singleâ€cluster catalysts: A new frontier in heterogeneous catalysis. Nano Select, 2021, 2, 251-270.	3.7	40
29	Assessment of Catalytic Activities of Gold Nanoclusters with Simple Structure Descriptors. ACS Catalysis, 2018, 8, 9702-9710.	11.2	38
30	Structures of small Pdâ€“Pt bimetallic clusters by Monte Carlo simulation. Chemical Physics, 2006, 330, 423-430.	1.9	37
31	One-pot synthesis of copperâ€“nickel sulfide nanowires for overall water splitting in alkaline media. Chemical Communications, 2019, 55, 8154-8157.	4.1	34
32	Structural transition and melting of onion-ring Pdâ€“Pt bimetallic clusters. Chemical Physics Letters, 2008, 461, 71-76.	2.6	33
33	Tuning the catalytic activity of Auâ€“Pd nanoalloys in CO oxidation via composition. Journal of Catalysis, 2014, 314, 47-55.	6.2	33
34	Biomass-derived porous carbon supported Co CoO yolk-shell nanoparticles as enhanced multifunctional electrocatalysts. International Journal of Hydrogen Energy, 2019, 44, 6525-6534.	7.1	33
35	Solid-State Synthesis of Highly Dispersed Nitrogen-Coordinated Single Iron Atom Electrocatalysts for Proton Exchange Membrane Fuel Cells. Nano Letters, 2021, 21, 3633-3639.	9.1	32
36	Understanding the structural properties and thermal stabilities of Auâ€“Pdâ€“Pt trimetallic clusters. Chemical Physics, 2014, 441, 152-158.	1.9	30

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37	Structures, Thermal Stability, and Chemical Activity of Crown-Jewel-Structured Pdâ€“Pt Nanoalloys. Journal of Physical Chemistry C, 2015, 119, 10888-10895.	3.1	29
38	Role of Composition and Geometric Relaxation in CO₂ Binding to Cuâ€“Ni Bimetallic Clusters. Journal of Physical Chemistry C, 2014, 118, 250-258.	3.1	26
39	Theoretical study of CO catalytic oxidation on free and defective graphene-supported Auâ€“Pd bimetallic clusters. RSC Advances, 2014, 4, 42554-42561.	3.6	26
40	Modification of the adsorption properties of O and OH on Ptâ€“Ni bimetallic surfaces by subsurface alloying. Electrochimica Acta, 2012, 76, 440-445.	5.2	25
41	Revisit the Role of Metal Dopants in Enhancing the Selectivity of Ag-Catalyzed Ethylene Epoxidation: Optimizing Oxophilicity of Reaction Site via Cocatalytic Mechanism. ACS Catalysis, 2021, 11, 3371-3383.	11.2	25
42	From mixed to three-layer core/shell PtCu nanoparticles: ligand-induced surface segregation to enhance electrocatalytic activity. Nanoscale, 2017, 9, 8945-8951.	5.6	24
43	Origin of enhanced ethylene oxide selectivity by Cs-promoted silver catalyst. Molecular Catalysis, 2017, 441, 92-99.	2.0	24
44	Mechanistic insight into the facet-dependent selectivity of ethylene epoxidation on Ag nanocatalysts. Applied Catalysis A: General, 2017, 538, 27-36.	4.3	22
45	Origin of Enhanced Activities for CO Oxidation and O₂ Reaction over Composition-Optimized Pd₅₀Cu₅₀ Nanoalloy Catalysts. Journal of Physical Chemistry C, 2017, 121, 11010-11020.	3.1	22
46	Enhancement Mechanism of the Conversion Effficiency of Dye-Sensitized Solar Cells Based on Nitrogen-, Fluorine-, and Iodine-Doped TiO₂ Photoanodes. Journal of Physical Chemistry C, 2015, 119, 13425-13432.	3.1	21
47	Hydrogen evolution reaction (HER) on Au@Ag ultrananoclusters as electro-catalysts. Nanoscale, 2018, 10, 17730-17737.	5.6	21
48	Oxygen-Reconstituted Active Species of Single-Atom Cu Catalysts for Oxygen Reduction Reaction. Research, 2020, 2020, 7593023.	5.7	21
49	Carbon-based material-supported single-atom catalysts for energy conversion. IScience, 2022, 25, 104367.	4.1	20
50	Structure, chemical ordering and thermal stability of Ptâ€“Ni alloy nanoclusters. Journal of Physics Condensed Matter, 2013, 25, 355008.	1.8	19
51	Shape-controlled Synthesis of PdCu Nanocrystals for Formic Acid Oxidation. Chemistry Letters, 2015, 44, 1101-1103.	1.3	19
52	PtCoNi Alloy Nanoclusters for Synergistic Catalytic Oxygen Reduction Reaction. ACS Applied Nano Materials, 2020, 3, 2536-2544.	5.0	18
53	Hydrogen generation from formic acid decomposition on Pdâ€“Cu nanoalloys. International Journal of Hydrogen Energy, 2019, 44, 24098-24109.	7.1	17
54	PdCu alloy nanoparticle-decorated copper nanotubes as enhanced electrocatalysts: DFT prediction validated by experiment. Nanotechnology, 2016, 27, 495403.	2.6	16

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55	Phase diagram and segregation of Agâ€“Co nanoalloys: insights from theory and simulation. Nanotechnology, 2016, 27, 115702.	2.6	15
56	Phase stability and segregation behavior of nickel-based nanoalloys based on theory and simulation. Journal of Alloys and Compounds, 2017, 708, 1150-1160.	5.5	15
57	Designing transition metal and nitrogen-codoped SrTiO₃(001) perovskite surfaces as efficient photocatalysts for water splitting. Sustainable Energy and Fuels, 2017, 1, 1968-1980.	4.9	15
58	Effect of Rhenium Loading Sequence on Selectivity of Agâ€“Cs Catalyst for Ethylene Epoxidation. Catalysis Letters, 2017, 147, 2920-2928.	2.6	14
59	Enhanced oxygen reduction activity of PtCu nanoparticles by morphology tuning and transition-metal doping. International Journal of Hydrogen Energy, 2020, 45, 4427-4434.	7.1	14
60	Ni (111)-supported graphene as a potential catalyst for high-efficient CO oxidation. Carbon, 2017, 116, 201-209.	10.3	13
61	Enhanced Ethylene Oxide Selectivity by Cu and Re Dual-Promoted Ag Catalysts. Industrial & Engineering Chemistry Research, 2018, 57, 4180-4185.	3.7	13
62	Individual Component Map of Rotatory Strength and Rotatory Strength Density Plots As Analysis Tools of Circular Dichroism Spectra of Complex Systems. Journal of Chemical Theory and Computation, 2018, 14, 3703-3714.	5.3	13
63	Understanding Hygroscopic Nucleation of Sulfate Aerosols: Combination of Molecular Dynamics Simulation with Classical Nucleation Theory. Journal of Physical Chemistry Letters, 2019, 10, 1126-1132.	4.6	13
64	Melting phenomena: effect of composition for 55-atom Agâ€“Pd bimetallic clusters. Physical Chemistry Chemical Physics, 2008, 10, 2513.	2.8	12
65	Revisit the Role of Chlorine in Selectivity Enhancement of Ethylene Epoxidation. Industrial & Engineering Chemistry Research, 2019, 58, 21403-21412.	3.7	11
66	Identification of the anti-triangular etched MoS2 with comparative activity with commercial Pt for hydrogen evolution reaction. International Journal of Hydrogen Energy, 2020, 45, 33457-33465.	7.1	11
67	Review on Synthesis and Catalytic Coupling Mechanism of Highly Active Electrocatalysts for Water Splitting. Energy Technology, 2021, 9, 2000855.	3.8	11
68	Bandgap engineering of MagnÃ©li phase TinO2nâˆ'1: Electron-hole self-compensation. Journal of Chemical Physics, 2015, 143, 054701.	3.0	10
69	Morphology Tailoring of Pt Nanocatalysts for the Oxygen Reduction Reaction: The Paradigm of Pt₁₃. ChemNanoMat, 2015, 1, 482-488.	2.8	10
70	Compositionâ€“controlled Synthesis of PtCuNPs Shells on Copper Nanowires as Electrocatalysts. ChemistrySelect, 2016, 1, 4392-4396.	1.5	10
71	Giant enhancement and anomalous temperature dependence of magnetism in monodispersed NiPt2 nanoparticles. Nano Research, 2017, 10, 3238-3247.	10.4	10
72	The Size Effect of PdCu Bimetallic Nanoparticles on Oxygen Reduction Reaction Activity. ChemElectroChem, 2018, 5, 2571-2576.	3.4	10

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73	Structure-controlled synthesis of one-dimensional PdCu nanoscatalysts via a seed-mediated approach for oxygen reduction reaction. Applied Surface Science, 2019, 493, 139-145.	6.1	10
74	Design of Highâ€Performance Coâ€Based Alloy Nanocatalysts for the Oxygen Reduction Reaction. Chemistry - A European Journal, 2020, 26, 4128-4135.	3.3	10
75	One-step synthesis of atomic Ru doped ultra-thin Co(OH)2 nanosheets for oxygen evolution reaction in different pH values. International Journal of Hydrogen Energy, 2021, 46, 22832-22841.	7.1	10
76	Concerted Catalysis on Tanghulu-like Cu@Zeolitic Imidazolate Framework-8 (ZIF-8) Nanowires with Tuning Catalytic Performances for 4-nitrophenol Reduction. Engineered Science, 2018, , .	2.3	10
77	Design of binary and ternary platinum shelled electrocatalysts with inexpensive metals for the oxygen reduction reaction. International Journal of Hydrogen Energy, 2016, 41, 13014-13023.	7.1	9
78	Promoter role of tungsten in W-Pd/Al2O3 catalyst for direct synthesis of H2O2: Modification of Pd/PdO ratio. Applied Catalysis A: General, 2021, 628, 118392.	4.3	9
79	CO oxidation mechanism on a MgO(1 0 0) supported Pt x Au 3â^'x clusters. Applied Surface Science, 2015, 356, 282-288.	6.1	8
80	Design of Single Atom Catalysts. Advances in Physics: X, 2021, 6, .	4.1	8
81	Constructing La-doped ultrathin Co-based nanostructured electrocatalysts for high-performance water oxidation process. International Journal of Hydrogen Energy, 2022, 47, 14504-14514.	7.1	7
82	Origin of enhanced stability and oxygen adsorption capacity of medium-sized Ptâ€"Ni nanoclusters. Journal of Physics Condensed Matter, 2018, 30, 285503.	1.8	6
83	Selectivity-Driven Design of the Agâ€"Cu Alloys for the Ethylene Epoxidation. Industrial & Engineering Chemistry Research, 2019, 58, 12996-13006.	3.7	5
84	Theoretical Study on the Structural, Thermal and Phase Stability of Ptâ€"Cu Alloy Clusters. Journal of Cluster Science, 2020, 31, 615-626.	3.3	5
85	Synergy in Auâ^'CuO Janus Structure for Catalytic Isopropanol Oxidative Dehydrogenation to Acetone. Angewandte Chemie, 2022, 134, .	2.0	5
86	Facet-dependent diffusion of atomic oxygen on Ag surfaces. Computational Materials Science, 2018, 155, 17-27.	3.0	4
87	Universal description of heating-induced reshaping preference of coreâ€"shell bimetallic nanoparticles. Nanoscale, 2019, 11, 1386-1395.	5.6	4
88	DFT Study of Pyrolysis Gasoline Hydrogenation on Pd(100), Pd(110) and Pd(111) Surfaces. Catalysis Letters, 2019, 149, 2226-2233.	2.6	3
89	Hydrogenase-Like Electrocatalytic Activation and Inactivation Mechanism by Three-Dimensional Binderless Molecular Catalyst. ACS Applied Energy Materials, 2019, 2, 3352-3362.	5.1	3
90	Effect of Size and Composition on the Structural Stability of Ptâ€"Ni Nanoalloys. Journal of Cluster Science, 2020, 31, 609-614.	3.3	2

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91	Magnetism in bimetallic PtxNiNâˆ’x clusters via cross-atomic coupling. Journal of Materials Chemistry C, 2019, 7, 9293-9300.	5.5	1