

Yan Zhao

List of Publications by Year in descending order

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227
papers

69,655
citations

8398

73
h-index

1429

214
g-index

231
all docs

231
docs citations

231
times ranked

41394
citing authors

#	ARTICLE	IF	CITATIONS
1	Tuning Structural and Electronic Configuration of $\langle \text{scp} \rangle \text{FeN}_4 \langle / \text{scp} \rangle$ via External S for Enhanced Oxygen Reduction Reaction. <i>Energy and Environmental Materials</i> , 2024, 7, .	13.2	9
2	The dual built-in electric fields across CoS/MoS ₂ heterojunctions for energy-saving hydrogen production coupled with sulfion degradation. <i>Journal of Colloid and Interface Science</i> , 2024, 657, 290-299.	9.7	7
3	Amorphous Sb/C composite with isotropic expansion property as an ultra-stable and high-rate anode for lithium-ion batteries. <i>Rare Metals</i> , 2024, 43, 2039-2052.	7.2	1
4	Boosting photocatalytic degradation of levofloxacin over plasmonic TiO ₂ -x/TiN heterostructure. <i>Applied Surface Science</i> , 2024, 655, 159516.	6.3	2
5	Iron Molybdenum Sulfideâ€‘Supported Ultrafine Ru Nanoclusters for Robust Sulfion Degradationâ€‘Assisted Hydrogen Production. <i>Advanced Functional Materials</i> , 2024, 34, .	16.4	2
6	Inâ€‘Situ Spontaneous Electropolymerization Enables Robust Hydrogel Electrolyte Interfaces in Aqueous Batteries. <i>Angewandte Chemie - International Edition</i> , 2024, 63, .	14.7	3
7	Inâ€‘Situ Spontaneous Electropolymerization Enables Robust Hydrogel Electrolyte Interfaces in Aqueous Batteries. <i>Angewandte Chemie</i> , 2024, 136, .	2.1	0
8	Potential-dependent activities in interpreting the reaction mechanism of dual-metal atom catalysts for Li-CO ₂ batteries. <i>Journal of Colloid and Interface Science</i> , 2024, 666, 276-284.	9.7	1
9	Theoretical Investigation of Nonmetallic Single-Atom Catalysts for Polysulfide Immobilization and Kinetic Enhancement in Lithiumâ€‘Sulfur Batteries. <i>Journal of Physical Chemistry C</i> , 2024, 128, 6551-6561.	3.3	0
10	Unveiling the Thermal Transitions of Silver Nanowires via In Situ TEM: Insights into Energy Transfer and Interfacial Stability. <i>Journal of Physical Chemistry C</i> , 2024, 128, 8270-8276.	3.3	0
11	Leveraging doping strategies and interface engineering to enhance catalytic transformation of lithium polysulfides for high-performance lithium-sulfur batteries. <i>Journal of Colloid and Interface Science</i> , 2024, 675, 904-914.	9.7	0
12	Enhancing photocatalytic CO ₂ reduction activity through Cobalt-Bismuth bimetallic Nanoparticle-Modified Nitrogen-Doped graphite carbon. <i>Journal of Colloid and Interface Science</i> , 2024, 675, 1069-1079.	9.7	0
13	Molecular Design Boosts Hydrolytic Stability of Diisopropanolamine Boronic Ester Hydrogel for Long-Term Drug Release. <i>Chemistry of Materials</i> , 2024, 36, 7232-7242.	7.0	0
14	Epitaxially Grown Ru Clustersâ€‘Nickel Nitride Heterostructure Advances Water Electrolysis Kinetics in Alkaline and Seawater Media. <i>Energy and Environmental Materials</i> , 2023, 6, .	13.2	59
15	Interfacial and Vacancies Engineering of Copper Nickel Sulfide for Enhanced Oxygen Reduction and Alcohols Oxidation Activity. <i>Energy and Environmental Materials</i> , 2023, 6, .	13.2	11
16	Three-dimensional palm frondlike Co ₃ O ₄ @NiO/graphitic carbon composite for photocatalytic CO ₂ reduction. <i>Journal of Alloys and Compounds</i> , 2023, 934, 168053.	5.7	10
17	3D porous flower-like CoAl ₂ O ₄ to boost the photocatalytic CO ₂ reduction reaction. <i>Journal of Materials Chemistry A</i> , 2023, 11, 2826-2835.	10.5	17
18	Multifunctional Multilayer Nanospheres for Ion Regulation in Lithium Metal Batteries. <i>Batteries</i> , 2023, 9, 149.	4.6	1

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19	Tailoring activity of iron phthalocyanine by edge-nitrogen sites induced electronic delocalization. <i>Applied Surface Science</i> , 2023, 624, 157154.	6.3	2
20	Boosting Oxygen Electrocatalytic Activity of Fe-N-C Catalysts by Phosphorus Incorporation. <i>Journal of the American Chemical Society</i> , 2023, 145, 3647-3655.	14.6	172
21	Dual Single-Atom Moieties Anchored on N-Doped Multilayer Graphene As a Catalytic Host for Lithium-Sulfur Batteries. <i>ACS Applied Materials & Interfaces</i> , 2023, 15, 9439-9446.	8.3	17
22	All-fluorinated electrolyte directly tuned Li ⁺ solvation sheath enabling high-quality passivated interfaces for robust Li metal battery under high voltage operation. <i>Energy Storage Materials</i> , 2023, 57, 249-259.	18.4	34
23	Engineering d-p orbital hybridization through regulation of interband energy separation for durable aqueous Zn/VO ₂ (B) batteries. <i>Chemical Engineering Journal</i> , 2023, 464, 142711.	13.0	18
24	A hydrated deep eutectic electrolyte with finely-tuned solvation chemistry for high-performance zinc-ion batteries. <i>Energy and Environmental Science</i> , 2023, 16, 2540-2549.	32.2	84
25	Bi ₂ MoO ₆ Embedded in 3D Porous N,O-Doped Carbon Nanosheets for Photocatalytic CO ₂ Reduction. <i>Nanomaterials</i> , 2023, 13, 1569.	4.2	3
26	Constructing Electrocatalysts with Composition Gradient Distribution by Solubility Product Theory: Amorphous/Crystalline CoNiFe-LDH Hollow Nanocages. <i>Advanced Functional Materials</i> , 2023, 33, .	16.4	18
27	Electronic and Vacancy Engineering of Mo-RuCoO _x Nanoarrays for High-Efficiency Water Splitting. <i>Advanced Functional Materials</i> , 2023, 33, .	16.4	22
28	Ultra-Uniform and Functionalized Nano-Ion Divider for Regulating Ion Distribution toward Dendrite-Free Lithium-Metal Batteries. <i>Advanced Materials</i> , 2023, 35, .	24.1	17
29	Effect of Major Factors on Lithium Dendrite Growth Studied by Phase Field Modeling. <i>Journal of the Electrochemical Society</i> , 2023, 170, 052506.	2.9	2
30	Constructing bimetallic heterostructure as anodes for sodium storage with superior stability and high capacity. <i>Journal of Power Sources</i> , 2023, 580, 233371.	8.0	3
31	Chip-based <i>in situ</i> TEM investigation of structural thermal instability in aged layered cathode. <i>Nanoscale Advances</i> , 2023, 5, 4182-4190.	4.6	0
32	Butyl ether as Co-diluent in medium-concentrated electrolyte for Li-S battery. <i>Journal of Energy Chemistry</i> , 2023, 85, 343-347.	13.4	0
33	High-Performance Sodium-Ion Batteries Enabled by 3D Nanoflowers Comprised of Ternary Sn-Based Dichalcogenides Embedded in Nitrogen and Sulfur Dual-Doped Carbon. <i>Small</i> , 2023, 19, .	11.1	7
34	Surface passivation for highly active, selective, stable, and scalable CO ₂ electroreduction. <i>Nature Communications</i> , 2023, 14, .	13.2	50
35	CdS-assisted ultrathin porous nitrogen-vacancy carbon nitride nanosheets for visible-light photocatalytic CO ₂ reduction. <i>Carbon</i> , 2023, 214, 118384.	10.7	4
36	Developing highly reversible Li- ² CO ₂ batteries: from on-chip exploration to practical application. <i>Energy and Environmental Science</i> , 2023, 16, 3960-3967.	32.2	5

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37	Crystal Engineering of Silica Anode Achieving Intrinsic Zero-Strain. <i>Advanced Materials</i> , 2023, 35, .	24.1	3
38	Transforming main-group elements into highly active single-atom electrocatalysts for oxygen reduction reactions. <i>Electrochimica Acta</i> , 2023, 469, 143223.	5.4	1
39	Metal-Organic Frameworks Nanocomposites with Different Dimensionalities for Energy Conversion and Storage. <i>Advanced Energy Materials</i> , 2022, 12, 2100346.	22.1	101
40	Density Functional Theory for Electrocatalysis. <i>Energy and Environmental Materials</i> , 2022, 5, 157-185.	13.2	133
41	Activating Inert Sites in Cobalt Silicate Hydroxides for Oxygen Evolution through Atomically Doping. <i>Energy and Environmental Materials</i> , 2022, 5, 655-661.	13.2	26
42	Facilitating the acidic oxygen reduction of Fe-N-C catalysts by fluorine-doping. <i>Materials Horizons</i> , 2022, 9, 417-424.	12.7	48
43	Combined enhanced redox kinetics and physiochemical confinement in three-dimensionally ordered macro/mesoporous TiN for highly stable lithium-sulfur batteries. <i>Nanotechnology</i> , 2022, 33, 115401.	2.7	2
44	A facile surface alloy-engineering route to enable robust lithium metal anodes. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 4751-4758.	2.9	8
45	Novel Two-Dimensional Metal-Based π -d Conjugated Nanosheets as Photocatalyst for Nitrogen Reduction Reaction: The First-Principle Investigation. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 5384-5394.	8.3	15
46	Core-shell Cu@Cu ₂ O nanoparticles embedded in 3D honeycomb-like N-doped graphitic carbon for photocatalytic CO ₂ reduction. <i>Journal of Materials Chemistry A</i> , 2022, 10, 4758-4769.	10.5	18
47	Tunable Ru ₂ P heterostructures with charge redistribution for efficient universal hydrogen evolution. <i>Informa-Materials</i> , 2022, 4, .	20.7	66
48	Interfacial gliding-driven lattice oxygen release in layered cathodes. <i>Cell Reports Physical Science</i> , 2022, 3, 100695.	5.8	5
49	Coordinatively Deficient Single-atom Fe-N-C Electrocatalyst with Optimized Electronic Structure for High-performance Lithium-sulfur Batteries. <i>Energy Storage Materials</i> , 2022, 46, 269-277.	18.4	119
50	Accurate redox potentials for solvents in Li-metal batteries and assessment of density functionals. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	2.1	7
51	The controlled in-situ growth of silver-halloysite nanostructure via interaction bonds to reinforce a novel polybenzoxazine composite resin and improve its antifouling and anticorrosion properties. <i>Composites Science and Technology</i> , 2022, 221, 109312.	8.0	8
52	Coordination environments tune the activity of oxygen catalysis on single atom catalysts: A computational study. <i>Nano Research</i> , 2022, 15, 3073-3081.	10.6	67
53	Theoretical insights into dual-atom catalysts for the oxygen reduction reaction: the crucial role of orbital polarization. <i>Journal of Materials Chemistry A</i> , 2022, 10, 9150-9160.	10.5	32
54	Electronic Regulation of ZnCo Dual-Atomic Active Sites Entrapped in 1D@2D Hierarchical N-Doped Carbon for Efficient Synergistic Catalysis of Oxygen Reduction in Zn-Air Battery. <i>Small</i> , 2022, 18, e2107141.	11.1	49

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55	Trimetallic Sulfide Hollow Superstructures with Engineered dâ€Band Center for Oxygen Reduction to Hydrogen Peroxide in Alkaline Solution. <i>Advanced Science</i> , 2022, 9, e2104768.	12.3	40
56	Trade-off effect of 3d transition metal doped boron nitride on anchoring polysulfides towards application in lithium-sulfur battery. <i>Journal of Colloid and Interface Science</i> , 2022, 616, 886-894.	9.7	8
57	Accelerating conversion of LiPSs on strain-induced MXene for high-performance Li-S battery. <i>Chemical Engineering Journal</i> , 2022, 439, 135679.	13.0	11
58	Stereoconvergent and stepwise 1,3-dipolar cycloadditions of nitrile oxides and nitrile imines. <i>Chinese Chemical Letters</i> , 2022, 33, 3012-3016.	9.1	8
59	Establishing a theoretical insight for penta-coordinated iron-nitrogen-carbon catalysts toward oxygen reaction. <i>Nano Research</i> , 2022, 15, 6067-6075.	10.6	44
60	Orthogonal State Reduction Variational Eigensolver for the Excited-State Calculations on Quantum Computers. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3737-3746.	5.6	11
61	Low-coordinated cobalt arrays for efficient hydrazine electrooxidation. <i>Energy and Environmental Science</i> , 2022, 15, 3246-3256.	32.2	48
62	A novel mixed ether-based electrolyte for lithiumâ€sulfur batteries with Li anode protection by dual salts. <i>Sustainable Energy and Fuels</i> , 2022, 6, 3658-3668.	4.8	6
63	Bioinspired mechanically interlocking holey graphene@SiO₂ anode. <i>Interdisciplinary Materials</i> , 2022, 1, 517-525.	14.7	53
64	High voltage and robust lithium metal battery enabled by highly-fluorinated interphases. <i>Energy Storage Materials</i> , 2022, 51, 317-326.	18.4	28
65	Qubit unitary coupled cluster with generalized single and paired double excitations ansatz for variational quantum eigensolver. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	2.1	2
66	Ultrahigh Stable Methanol Oxidation Enabled by a High Hydroxyl Concentration on Pt Clusters/MXene Interfaces. <i>Journal of the American Chemical Society</i> , 2022, 144, 15529-15538.	14.6	172
67	Strategy to weaken the oxygen adsorption on single-atom catalysts towards oxygen-involved reactions. <i>Materials Today Advances</i> , 2022, 16, 100280.	5.5	5
68	CoFe alloy nanoparticles encapsulated in a 3D honeycomb-like N-doped graphitic carbon framework for photocatalytic CO₂ reduction. <i>Journal of Materials Chemistry A</i> , 2022, 10, 22093-22104.	10.5	12
69	Machine learning for battery research. <i>Journal of Power Sources</i> , 2022, 549, 232125.	8.0	37
70	A paradigm for systematic screening and evaluation of artificial solid-electrolyte interfaces for lithium metal anodes: a computational study of binary selenides. <i>Journal of Materials Chemistry A</i> , 2022, 10, 24226-24237.	10.5	2
71	A new ether-based medium-concentrated electrolyte for lithiumâ€sulfur battery with lean Li anode. <i>Journal of Power Sources</i> , 2022, 551, 232211.	8.0	11
72	Hydrofluoroether Diluted Dualâ€Saltsâ€Based Electrolytes for Lithiumâ€Sulfur Batteries with Enhanced Lithium Anode Protection. <i>Small</i> , 2022, 18, .	11.1	8

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73	A solid-state Matryoshka doll-like microwave method for one-step rapid synthesis of composites of NiSe ₂ and nitrogen-doped porous carbon for sodium storage. <i>Journal of Materials Chemistry C</i> , 2022, 10, 18052-18062.	5.6	7
74	Operando Observation of Coupled Discontinuous-Continuous Transitions in Ion-Stabilized Intercalation Cathodes. <i>Batteries</i> , 2022, 8, 252.	4.6	2
75	Power of the Sine Hamiltonian Operator for Estimating the Eigenstate Energies on Quantum Computers. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 7586-7602.	5.6	3
76	Facet-Dependent Oxygen Reduction Reaction Activity on the Surfaces of Co ₃ O ₄ . <i>Energy and Environmental Materials</i> , 2021, 4, 407-412.	13.2	21
77	Nano-Ferric Oxide Embedded in Graphene Oxide: High-performance Electrocatalyst for Nitrogen Reduction at Ambient Condition. <i>Energy and Environmental Materials</i> , 2021, 4, 88-94.	13.2	48
78	First-principles investigations on the synergistic effect of N-dopant and lattice-strain for CO ₂ reduction to CO on graphene. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26535.	2.1	0
79	Structural properties and electrochemical performance of different polymorphs of Nb ₂ O ₅ in magnesium-based batteries. <i>Journal of Energy Chemistry</i> , 2021, 58, 586-592.	13.4	14
80	Computational Design of Single Mo Atom Anchored Defective Boron Phosphide Monolayer as a High-performance Electrocatalyst for the Nitrogen Reduction Reaction. <i>Energy and Environmental Materials</i> , 2021, 4, 255-262.	13.2	36
81	Novel graphitic carbon nitride g-C ₉ N ₁₀ as a promising platform to design efficient photocatalysts for dinitrogen reduction to ammonia: the first-principles investigation. <i>Journal of Materials Chemistry A</i> , 2021, 9, 20615-20625.	10.5	26
82	Significantly enhancing the dielectric constant and breakdown strength of linear dielectric polymers by utilizing ultralow loadings of nanofillers. <i>Journal of Materials Chemistry A</i> , 2021, 9, 23028-23036.	10.5	67
83	Zn-Co Zeolitic Imidazolate Framework Nanoparticles Intercalated in Graphene Nanosheets for Room-Temperature NO ₂ Sensing. <i>ACS Applied Nano Materials</i> , 2021, 4, 3998-4006.	5.2	16
84	High Yield Electrosynthesis of Hydrogen Peroxide from Water Using Electrospun CaSnO ₃ @Carbon Fiber Membrane Catalysts with Abundant Oxygen Vacancy. <i>Advanced Functional Materials</i> , 2021, 31, 2100099.	16.4	57
85	Atomistic Modeling of PEDOT:PSS Complexes I: DFT Benchmarking. <i>Macromolecules</i> , 2021, 54, 3634-3646.	5.1	18
86	Interface cation migration kinetics induced oxygen release heterogeneity in layered lithium cathodes. <i>Energy Storage Materials</i> , 2021, 36, 115-122.	18.4	25
87	Quicker and More Zn ²⁺ Storage Predominantly from the Interface. <i>Advanced Materials</i> , 2021, 33, e2100359.	24.1	124
88	Active Site Identification and Interfacial Design of a MoP/N-Doped Carbon Catalyst for Efficient Hydrogen Evolution Reaction. <i>ACS Applied Energy Materials</i> , 2021, 4, 5486-5492.	5.3	19
89	Atomic-Level Modulation of the Interface Chemistry of Platinum-Nickel Oxide toward Enhanced Hydrogen Electrocatalysis Kinetics. <i>Nano Letters</i> , 2021, 21, 4845-4852.	9.5	39
90	Atomistic Modeling of PEDOT:PSS Complexes II: Force Field Parameterization. <i>Macromolecules</i> , 2021, 54, 5354-5365.	5.1	13

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91	Revealing the Multi-Electron Reaction Mechanism of $\text{Na}_3\text{V}_2\text{O}_8(\text{PO}_4)_2\text{F}$ Towards Improved Lithium Storage. <i>ChemSusChem</i> , 2021, 14, 2984-2991.	7.4	10
92	Diastereodivergent 1,3-Dipolar Cycloaddition of β -Fluoro- α,β -Unsaturated Arylketones and Azomethine Ylides: Experimental and Theoretical DFT Studies. <i>European Journal of Organic Chemistry</i> , 2021, 2021, 5530-5535.	2.5	7
93	Significant Improvements in Dielectric Constant and Energy Density of Ferroelectric Polymer Nanocomposites Enabled by Ultralow Contents of Nanofillers. <i>Advanced Materials</i> , 2021, 33, e2102392.	24.1	118
94	Computational investigation of 2D 3d/4d hexagonal transition metal borides for metal-ion batteries. <i>Electrochimica Acta</i> , 2021, 384, 138404.	5.4	19
95	Rational design of a cobalt sulfide nanoparticle-embedded flexible carbon nanofiber membrane electrocatalyst for advanced lithium-sulfur batteries. <i>Nanotechnology</i> , 2021, 32, 455703.	2.7	4
96	Additive kinematic formulas for flag area measures. <i>Mathematische Annalen</i> , 2021, 381, 1615-1652.	1.5	1
97	Exploring the anchoring effect and catalytic mechanism of 3d transition metal phthalocyanine for S8/LiPSs: A density functional theory study. <i>Applied Surface Science</i> , 2021, 558, 149928.	6.3	22
98	β -Be water strategy of liquid lithium sulfide enables 0.2 V potential barrier for high-performance lithium-sulfur batteries. <i>Materials Today Energy</i> , 2021, 21, 100793.	5.2	10
99	Suppressing Polysulfide Shuttling in Lithium-Sulfur Batteries via a Multifunctional Conductive Binder. <i>Small Methods</i> , 2021, 5, e2100839.	9.6	15
100	Gradient sulfur fixing separator with catalytic ability for stable lithium sulfur battery. <i>Chemical Engineering Journal</i> , 2021, 422, 130107.	13.0	40
101	Gradient SEI layer induced by liquid alloy electrolyte additive for high rate lithium metal battery. <i>Nano Energy</i> , 2021, 88, 106237.	16.5	59
102	Highly active Fe centered FeM-N-doped carbon (M=Co/Ni/Mn): A general strategy for efficient oxygen conversion in Zn-air battery. <i>Chemical Engineering Journal</i> , 2021, 424, 130559.	13.0	58
103	Development of a curcumin-based antifouling and anticorrosion sustainable polybenzoxazine resin composite coating. <i>Composites Part B: Engineering</i> , 2021, 225, 109263.	12.2	63
104	Virtual screening of two-dimensional selenides and transition metal doped SnSe for lithium-sulfur batteries: A first-principles study. <i>Applied Surface Science</i> , 2021, 570, 151213.	6.3	42
105	Three-dimensional porous N-doped graphitic carbon framework with embedded CoO for photocatalytic CO ₂ reduction. <i>Applied Catalysis B: Environmental</i> , 2021, 298, 120546.	20.7	46
106	Accurate correlation energy functional for uniform electron gas from an interpolation ansatz without fitting parameters. <i>Physical Review B</i> , 2021, 103, .	3.3	2
107	Strain Engineering of a MXene/CNT Hierarchical Porous Hollow Microsphere Electrocatalyst for a High-Efficiency Lithium Polysulfide Conversion Process. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 2371-2378.	14.7	195
108	Interfacial interaction-induced temperature-dependent mechanical property of graphene-PDMS nanocomposite. <i>Journal of Materials Science</i> , 2020, 55, 1553-1561.	3.7	18

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109	Low-Bandgap Se-Deficient Antimony Selenide as a Multifunctional Polysulfide Barrier toward High-Performance Lithium-Sulfur Batteries. <i>Advanced Materials</i> , 2020, 32, e1904876.	24.1	217
110	Interface enhanced well-dispersed Co ₉ S ₈ nanocrystals as an efficient polysulfide host in lithium-sulfur batteries. <i>Journal of Energy Chemistry</i> , 2020, 48, 109-115.	13.4	61
111	A flexible, hierarchically porous PANI/MnO ₂ network with fast channels and an extraordinary chemical process for stable fast-charging lithium-sulfur batteries. <i>Journal of Materials Chemistry A</i> , 2020, 8, 2741-2751.	10.5	54
112	MXene Surface Terminations Enable Strong Metal-Support Interactions for Efficient Methanol Oxidation on Palladium. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 2400-2406.	8.3	85
113	Transition metals doped borophene-graphene heterostructure for robust polysulfide anchoring: A first principle study. <i>Applied Surface Science</i> , 2020, 534, 147575.	6.3	22
114	Soft on rigid nanohybrid as the self-supporting multifunctional cathode electrocatalyst for high-performance lithium-polysulfide batteries. <i>Nano Energy</i> , 2020, 78, 105293.	16.5	39
115	Multilayer stabilization for fabricating high-loading single-atom catalysts. <i>Nature Communications</i> , 2020, 11, 5892.	13.2	225
116	Ru-doped 3D flower-like bimetallic phosphide with a climbing effect on overall water splitting. <i>Applied Catalysis B: Environmental</i> , 2020, 279, 119396.	20.7	289
117	Modulation of J-Aggregation of Nonfullerene Acceptors toward Near-Infrared Absorption and Enhanced Efficiency. <i>Macromolecules</i> , 2020, 53, 3747-3755.	5.1	40
118	Oxygen defects boost polysulfides immobilization and catalytic conversion: First-principles computational characterization and experimental design. <i>Nano Research</i> , 2020, 13, 2299-2307.	10.6	41
119	NWChem: Past, present, and future. <i>Journal of Chemical Physics</i> , 2020, 152, 184102.	3.1	479
120	A three-dimensional nitrogen-doped graphene framework decorated with an atomic layer deposited ultrathin V ₂ O ₅ layer for lithium sulfur batteries with high sulfur loading. <i>Journal of Materials Chemistry A</i> , 2020, 8, 12106-12113.	10.5	30
121	Polymer dielectrics exhibiting an anomalously improved dielectric constant simultaneously achieved high energy density and efficiency enabled by CdSe/Cd _{1-x} Zn _x S quantum dots. <i>Journal of Materials Chemistry A</i> , 2020, 8, 13659-13670.	10.5	25
122	Multi-coefficients correlation methods. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2020, 10, e1474.	16.3	4
123	All-Purpose Electrode Design of Flexible Conductive Scaffold toward High-Performance Li-S Batteries. <i>Advanced Functional Materials</i> , 2020, 30, 2000613.	16.4	97
124	Three-Dimensional Porous Nitrogen-Doped Carbon Nanosheet with Embedded Ni ₃ Co ₃ S ₄ Nanocrystals for Advanced Lithium-Sulfur Batteries. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 9181-9189.	8.3	42
125	Fluorinated solid additives enable high efficiency non-fullerene organic solar cells. <i>Journal of Materials Chemistry A</i> , 2020, 8, 4230-4238.	10.5	52
126	Multistep Reaction Pathway for CO ₂ Reduction on Hydride-Capped Si Nanosheets. <i>ChemCatChem</i> , 2020, 12, 722-725.	3.8	1

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127	A robust electrospun separator modified with in situ grown metal-organic frameworks for lithium-sulfur batteries. <i>Chemical Engineering Journal</i> , 2020, 395, 124979.	13.0	95
128	Facile formation of tetragonal-Nb ₂ O ₅ microspheres for high-rate and stable lithium storage with high areal capacity. <i>Science Bulletin</i> , 2020, 65, 1154-1162.	11.1	66
129	High-Voltage Cycling Induced Thermal Vulnerability in LiCoO ₂ Cathode: Cation Loss and Oxygen Release Driven by Oxygen Vacancy Migration. <i>ACS Nano</i> , 2020, 14, 6181-6190.	15.2	165
130	Diastereodivergent Asymmetric 1,3-Dipolar Cycloaddition of Azomethine Ylides and β -Fluoroalkyl Vinylsulfones: Low Copper(II) Catalyst Loading and Theoretical Studies. <i>Angewandte Chemie</i> , 2019, 131, 16790-16796.	2.1	10
131	Diastereodivergent Asymmetric 1,3-Dipolar Cycloaddition of Azomethine Ylides and β -Fluoroalkyl Vinylsulfones: Low Copper(II) Catalyst Loading and Theoretical Studies. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 16637-16643.	14.7	48
132	1,2-Amino alcohol-dependent Petasis allylboration for racemic and chiral homoallylamines. <i>Organic Chemistry Frontiers</i> , 2019, 6, 751-755.	4.6	15
133	Uniform zeolitic imidazolate framework coating via in situ recoordination for efficient polysulfide trapping. <i>Energy Storage Materials</i> , 2019, 23, 55-61.	18.4	34
134	Construction of Oxygen-Deficient La(OH) ₃ Nanorods Wrapped by Reduced Graphene Oxide for Polysulfide Trapping toward High-Performance Lithium/Sulfur Batteries. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 23271-23279.	8.3	73
135	Identification of Phase Control of Carbon-Confined Nb ₂ O ₅ Nanoparticles toward High-Performance Lithium Storage. <i>Advanced Energy Materials</i> , 2019, 9, 1802695.	22.1	169
136	Density Functional Theory for Battery Materials. <i>Energy and Environmental Materials</i> , 2019, 2, 264-279.	13.2	237
137	Revealing the atomistic origin of the disorder-enhanced Na-storage performance in NaFePO ₄ battery cathode. <i>Nano Energy</i> , 2019, 57, 608-615.	16.5	76
138	Extrapolation of high-order correlation energies: the WMS model. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 27375-27384.	2.9	39
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