

Yan Zhao

List of Publications by Year in descending order

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160
papers

65,889
citations

11651

70
h-index

5988

160
g-index

163
all docs

163
docs citations

163
times ranked

40123
citing authors

#	ARTICLE	IF	CITATIONS
1	The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 215-241.	1.4	23,928
2	Density Functionals with Broad Applicability in Chemistry. <i>Accounts of Chemical Research</i> , 2008, 41, 157-167.	15.6	6,193
3	A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions. <i>Journal of Chemical Physics</i> , 2006, 125, 194101.	3.0	4,175
4	Design of Density Functionals by Combining the Method of Constraint Satisfaction with Parametrization for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 364-382.	5.3	3,329
5	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	1.7	2,561
6	Hybrid Meta Density Functional Theory Methods for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions: The MPW1B95 and MPWB1K Models and Comparative Assessments for Hydrogen Bonding and van der Waals Interactions. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6908-6918.	2.5	1,497
7	Design of Density Functionals That Are Broadly Accurate for Thermochemistry, Thermochemical Kinetics, and Nonbonded Interactions. <i>Journal of Physical Chemistry A</i> , 2005, 109, 5656-5667.	2.5	1,451
8	Computational Thermochemistry: Scale Factor Databases and Scale Factors for Vibrational Frequencies Obtained from Electronic Model Chemistries. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2872-2887.	5.3	1,183
9	Density Functional for Spectroscopy: A No Long-Range Self-Interaction Error, Good Performance for Rydberg and Charge-Transfer States, and Better Performance on Average than B3LYP for Ground States. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13126-13130.	2.5	1,140
10	Exchange-correlation functional with broad accuracy for metallic and nonmetallic compounds, kinetics, and noncovalent interactions. <i>Journal of Chemical Physics</i> , 2005, 123, 161103.	3.0	979
11	Exploring the Limit of Accuracy of the Global Hybrid Meta Density Functional for Main-Group Thermochemistry, Kinetics, and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1849-1868.	5.3	956
12	Twinborn TiO ₂ TiN heterostructures enabling smooth trapping of polysulfides towards ultralong life lithium-sulfur batteries. <i>Energy and Environmental Science</i> , 2017, 10, 1694-1703.	30.8	884
13	Benchmark Databases for Nonbonded Interactions and Their Use To Test Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 415-432.	5.3	832
14	Benchmark Database of Barrier Heights for Heavy Atom Transfer, Nucleophilic Substitution, Association, and Unimolecular Reactions and Its Use to Test Theoretical Methods. <i>Journal of Physical Chemistry A</i> , 2005, 109, 2012-2018.	2.5	736
15	Comparative DFT Study of van der Waals Complexes: Rare-Gas Dimers, Alkaline-Earth Dimers, Zinc Dimer, and Zinc-Rare-Gas Dimers. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5121-5129.	2.5	706
16	Effectiveness of Diffuse Basis Functions for Calculating Relative Energies by Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1384-1388.	2.5	688
17	Applications and validations of the Minnesota density functionals. <i>Chemical Physics Letters</i> , 2011, 502, 1-13.	2.6	662
18	Development and Assessment of a New Hybrid Density Functional Model for Thermochemical Kinetics. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2715-2719.	2.5	639

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19	Density Functionals for Noncovalent Interaction Energies of Biological Importance. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 289-300.	5.3	557
20	The DBH24/08 Database and Its Use to Assess Electronic Structure Model Chemistries for Chemical Reaction Barrier Heights. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 808-821.	5.3	462
21	Density Functionals for Inorganometallic and Organometallic Chemistry. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11127-11143.	2.5	447
22	NWChem: Past, present, and future. <i>Journal of Chemical Physics</i> , 2020, 152, 184102.	3.0	425
23	Multi-coefficient extrapolated density functional theory for thermochemistry and thermochemical kinetics. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 43.	2.8	393
24	On the Performances of the M06 Family of Density Functionals for Electronic Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2071-2085.	5.3	383
25	How Well Can New-Generation Density Functionals Describe the Energetics of Bond-Dissociation Reactions Producing Radicals?. <i>Journal of Physical Chemistry A</i> , 2008, 112, 1095-1099.	2.5	359
26	Lithiophilic-lithiophobic gradient interfacial layer for a highly stable lithium metal anode. <i>Nature Communications</i> , 2018, 9, 3729.	12.8	331
27	Benchmark Energetic Data in a Model System for Grubbs II Metathesis Catalysis and Their Use for the Development, Assessment, and Validation of Electronic Structure Methods. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 324-333.	5.3	313
28	Doubly Hybrid Meta DFT: A New Multi-Coefficient Correlation and Density Functional Methods for Thermochemistry and Thermochemical Kinetics. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4786-4791.	2.5	297
29	Construction of a generalized gradient approximation by restoring the density-gradient expansion and enforcing a tight Lieb-Oxford bound. <i>Journal of Chemical Physics</i> , 2008, 128, 184109.	3.0	260
30	A 3D Nitrogen-Doped Graphene/TiN Nanowires Composite as a Strong Polysulfide Anchor for Lithium-Sulfur Batteries with Enhanced Rate Performance and High Areal Capacity. <i>Advanced Materials</i> , 2018, 30, e1804089.	21.0	251
31	Ru-doped 3D flower-like bimetallic phosphide with a climbing effect on overall water splitting. <i>Applied Catalysis B: Environmental</i> , 2020, 279, 119396.	20.2	251
32	How well can new-generation density functional methods describe stacking interactions in biological systems?. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 2701.	2.8	246
33	Tests of second-generation and third-generation density functionals for thermochemical kinetics. Electronic supplementary information (ESI) available: Mean errors for pure and hybrid DFT methods. See http://www.rsc.org/suppdata/cp/b3/b316260e/ . <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 673.	2.8	242
34	Computational characterization and modeling of buckyball tweezers: density functional study of concave-convex interactions. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 2813.	2.8	218
35	Assessment of Model Chemistries for Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1009-1018.	5.3	214
36	Databases for Transition Element Bonding: Metal-Metal Bond Energies and Bond Lengths and Their Use To Test Hybrid, Hybrid Meta, and Meta Density Functionals and Generalized Gradient Approximations. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4388-4403.	2.5	209

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37	Representative Benchmark Suites for Barrier Heights of Diverse Reaction Types and Assessment of Electronic Structure Methods for Thermochemical Kinetics. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 569-582.	5.3	207
38	Tests of the RPBE, revPBE, ĩ,-HCTHhyb, ĩ%B97X-D, and MOHLYP density functional approximations and 29 others against representative databases for diverse bond energies and barrier heights in catalysis. <i>Journal of Chemical Physics</i> , 2010, 132, 164117.	3.0	206
39	Low Bandgap Se Deficient Antimony Selenide as a Multifunctional Polysulfide Barrier toward High Performance Lithium Sulfur Batteries. <i>Advanced Materials</i> , 2020, 32, e1904876.	21.0	206
40	Assessment of Density Functionals for ĩ Systems: Energy Differences between Cumulenes and Polyynes; Proton Affinities, Bond Length Alternation, and Torsional Potentials of Conjugated Polyenes; and Proton Affinities of Conjugated Schiff Bases. <i>Journal of Physical Chemistry A</i> , 2006, 110, 10478-10486.	2.5	196
41	Multilayer stabilization for fabricating high-loading single-atom catalysts. <i>Nature Communications</i> , 2020, 11, 5892.	12.8	195
42	A Density Functional That Accounts for Medium-Range Correlation Energies in Organic Chemistry. <i>Organic Letters</i> , 2006, 8, 5753-5755.	4.6	193
43	Density Functional Theory for Reaction Energies: Test of Meta and Hybrid Meta Functionals, Range-Separated Functionals, and Other High-Performance Functionals. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 669-676.	5.3	190
44	Density Functional Theory for Battery Materials. <i>Energy and Environmental Materials</i> , 2019, 2, 264-279.	12.8	186
45	Comparative assessment of density functional methods for 3d transition-metal chemistry. <i>Journal of Chemical Physics</i> , 2006, 124, 224105.	3.0	180
46	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.	13.8	176
47	Generalized Gradient Approximation That Recovers the Second-Order Density-Gradient Expansion with Optimized Across-the-Board Performance. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 1991-1997.	4.6	171
48	How Well Can Density Functional Methods Describe Hydrogen Bonds to ĩ Acceptors?. <i>Journal of Physical Chemistry B</i> , 2005, 109, 19046-19051.	2.6	169
49	Attractive Noncovalent Interactions in the Mechanism of Grubbs Second-Generation Ru Catalysts for Olefin Metathesis. <i>Organic Letters</i> , 2007, 9, 1967-1970.	4.6	163
50	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.	19.5	161
51	Benchmark Data for Interactions in Zeolite Model Complexes and Their Use for Assessment and Validation of Electronic Structure Methods. <i>Journal of Physical Chemistry C</i> , 2008, 112, 6860-6868.	3.1	157
52	A Prototype for Graphene Material Simulation: Structures and Interaction Potentials of Coronene Dimers. <i>Journal of Physical Chemistry C</i> , 2008, 112, 4061-4067.	3.1	152
53	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.	14.6	144
54	The 6-31B(d) Basis Set and the BMC-QCISD and BMC-CCSD Multicoefficient Correlation Methods. <i>Journal of Physical Chemistry A</i> , 2005, 109, 1643-1649.	2.5	138

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55	Verdict: Time-Dependent Density Functional Theory "Not Guilty" of Large Errors for Cyanines. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1255-1259.	5.3	122
56	Thermochemical Kinetics for Multireference Systems: Addition Reactions of Ozone. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5786-5799.	2.5	114
57	Quicker and More Zn ²⁺ Storage Predominantly from the Interface. <i>Advanced Materials</i> , 2021, 33, e2100359.	21.0	111
58	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.	21.0	102
59	Multicoefficient Extrapolated Density Functional Theory Studies of $\pi\text{-}\pi$ Interactions: The Benzene Dimer. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4209-4212.	2.5	99
60	Density Functional Theory for Electrocatalysis. <i>Energy and Environmental Materials</i> , 2022, 5, 157-185.	12.8	95
61	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.	18.0	95
62	Improved Description of Nuclear Magnetic Resonance Chemical Shielding Constants Using the M06-L Meta-Generalized-Gradient-Approximation Density Functional. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6794-6799.	2.5	92
63	All-Purpose Electrode Design of Flexible Conductive Scaffold toward High-Performance Li-S Batteries. <i>Advanced Functional Materials</i> , 2020, 30, 2000613.	14.9	90
64	Infinite-Basis Calculations of Binding Energies for the Hydrogen Bonded and Stacked Tetramers of Formic Acid and Formamide and Their Use for Validation of Hybrid DFT and ab Initio Methods. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6624-6627.	2.5	89
65	Size-Selective Supramolecular Chemistry in a Hydrocarbon Nanoring. <i>Journal of the American Chemical Society</i> , 2007, 129, 8440-8442.	13.7	89
66	Metal-Organic Frameworks Nanocomposites with Different Dimensionalities for Energy Conversion and Storage. <i>Advanced Energy Materials</i> , 2022, 12, 2100346.	19.5	86
67	A robust electrospun separator modified with in situ grown metal-organic frameworks for lithium-sulfur batteries. <i>Chemical Engineering Journal</i> , 2020, 395, 124979.	12.7	85
68	Validation of electronic structure methods for isomerization reactions of large organic molecules. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 13683.	2.8	78
69	Calculation of semiconductor band gaps with the M06-L density functional. <i>Journal of Chemical Physics</i> , 2009, 130, 074103.	3.0	75
70	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.	8.0	71
71	Revealing the atomistic origin of the disorder-enhanced Na-storage performance in NaFePO ₄ battery cathode. <i>Nano Energy</i> , 2019, 57, 608-615.	16.0	67
72	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.	9.0	64

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73	Improved CO Adsorption Energies, Site Preferences, and Surface Formation Energies from a Meta-Generalized Gradient Approximation Exchange-Correlation Functional, M06-L. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2975-2979.	4.6	63
74	Benchmark Database for Ylidic Bond Dissociation Energies and Its Use for Assessments of Electronic Structure Methods. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2824-2834.	5.3	62
75	Benchmarking approximate density functional theory for s/d excitation energies in 3d transition metal cations. <i>Journal of Computational Chemistry</i> , 2008, 29, 185-189.	3.3	61
76	Thermochemical Kinetics of Hydrogen-Atom Transfers between Methyl, Methane, Ethynyl, Ethyne, and Hydrogen. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4632-4642.	2.5	59
77	Carbene Rotamer Switching Explains the Reverse Trans Effect in Forming the Grubbs Second-Generation Olefin Metathesis Catalyst. <i>Organometallics</i> , 2011, 30, 4196-4200.	2.3	59
78	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.	12.9	59
79	Coordination environments tune the activity of oxygen catalysis on single atom catalysts: A computational study. <i>Nano Research</i> , 2022, 15, 3073-3081.	10.4	58
80	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.	12.7	55
81	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.	10.3	54
82	Tunable Ru ₂ P heterostructures with charge redistribution for efficient universal hydrogen evolution. <i>Information Materials</i> , 2022, 4, .	17.3	53
83	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.	14.9	52
84	Development of a curcumin-based antifouling and anticorrosion sustainable polybenzoxazine resin composite coating. <i>Composites Part B: Engineering</i> , 2021, 225, 109263.	12.0	51
85	Binding energy of d10 transition metals to alkenes by wave function theory and density functional theory†. <i>Journal of Molecular Catalysis A</i> , 2010, 324, 80-88.	4.8	50
86	Gradient SEI layer induced by liquid alloy electrolyte additive for high rate lithium metal battery. <i>Nano Energy</i> , 2021, 88, 106237.	16.0	48
87	Combined valence bond-molecular mechanics potential-energy surface and direct dynamics study of rate constants and kinetic isotope effects for the H+C ₂ H ₆ reaction. <i>Journal of Chemical Physics</i> , 2006, 124, 044315.	3.0	47
88	Density Functional Calculations of E ₂ and S _N ² Reactions: Effects of the Choice of Density Functional, Basis Set, and Self-Consistent Iterations. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1104-1108.	5.3	45
89	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.	12.8	44
90	Diastereodivergent Asymmetric 1,3-Dipolar Cycloaddition of Azomethine Ylides and Fluoroalkyl Vinylsulfones: Low Copper(II) Catalyst Loading and Theoretical Studies. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 16637-16643.	13.8	43

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91	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.	20.2	42
92	Bioinspired mechanically interlocking holey graphene@SiO ₂ anode. , 2022, 1, 517-525.		42
93	How Well Can New-Generation Density Functionals Describe Protonated Epoxides Where Older Functionals Fail?. <i>Journal of Organic Chemistry</i> , 2007, 72, 295-298.	3.2	41
94	Effect of Triton X-100 on the stability of aqueous dispersions of copper phthalocyanine pigment nanoparticles. <i>Journal of Colloid and Interface Science</i> , 2011, 362, 33-41.	9.4	40
95	Facilitating the acidic oxygen reduction of Fe-N-C catalysts by fluorine-doping. <i>Materials Horizons</i> , 2022, 9, 417-424.	12.2	39
96	Multiconfiguration Molecular Mechanics Based on Combined Quantum Mechanical and Molecular Mechanical Calculations. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1237-1254.	5.3	38
97	Soft on rigid nano-hybrid as the self-supporting multifunctional cathode electrocatalyst for high-performance lithium-polysulfide batteries. <i>Nano Energy</i> , 2020, 78, 105293.	16.0	36
98	Oxygen defects boost polysulfides immobilization and catalytic conversion: First-principles computational characterization and experimental design. <i>Nano Research</i> , 2020, 13, 2299-2307.	10.4	36
99	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.	8.0	36
100	Gradient sulfur fixing separator with catalytic ability for stable lithium sulfur battery. <i>Chemical Engineering Journal</i> , 2021, 422, 130107.	12.7	36
101	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.	6.1	36
102	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.	10.0	36
103	Low-coordinated cobalt arrays for efficient hydrazine electrooxidation. <i>Energy and Environmental Science</i> , 2022, 15, 3246-3256.	30.8	36
104	The Minnesota Density Functionals and their Applications to Problems in Mineralogy and Geochemistry. <i>Reviews in Mineralogy and Geochemistry</i> , 2010, 71, 19-37.	4.8	35
105	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.	12.8	35
106	Extrapolation of high-order correlation energies: the WMS model. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 27375-27384.	2.8	34
107	Accurate Binding Energies for Lithium Polysulfides and Assessment of Density Functionals for Lithium-Sulfur Battery Research. <i>Journal of Physical Chemistry C</i> , 2019, 123, 20737-20747.	3.1	34
108	Uniform zeolitic imidazolate framework coating via in situ recoordination for efficient polysulfide trapping. <i>Energy Storage Materials</i> , 2019, 23, 55-61.	18.0	33

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109	Atomic-Level Modulation of the Interface Chemistry of Platinum–Nickel Oxide toward Enhanced Hydrogen Electrocatalysis Kinetics. <i>Nano Letters</i> , 2021, 21, 4845-4852.	9.1	31
110	Multicoefficient Gaussian-3 Calculation of the Rate Constant for the OH + CH ₄ Reaction and Its ¹² C/ ¹³ C Kinetic Isotope Effect with Emphasis on the Effects of Coordinate System and Torsional Treatment. <i>Journal of Physical Chemistry A</i> , 2007, 111, 11706-11717.	2.5	30
111	Benchmark Data for Noncovalent Interactions in HCOOH–Benzene Complexes and Their Use for Validation of Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2726-2733.	5.3	30
112	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.	10.3	28
113	Establishing a theoretical insight for penta-coordinated iron-nitrogen-carbon catalysts toward oxygen reaction. <i>Nano Research</i> , 2022, 15, 6067-6075.	10.4	28
114	Trimetallic Sulfide Hollow Superstructures with Engineered d-Band Center for Oxygen Reduction to Hydrogen Peroxide in Alkaline Solution. <i>Advanced Science</i> , 2022, 9, e2104768.	11.2	26
115	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.	10.3	25
116	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.	10.3	25
117	Comment on “More accurate generalized gradient approximation for solids”. <i>Physical Review B</i> , 2008, 78, .	3.2	24
118	Colloidal Dispersion Stability of CuPc Aqueous Dispersions and Comparisons to Predictions of the DLVO Theory for Spheres and Parallel Face-to-Face Cubes. <i>Langmuir</i> , 2010, 26, 6995-7006.	3.5	23
119	Interface cation migration kinetics induced oxygen release heterogeneity in layered lithium cathodes. <i>Energy Storage Materials</i> , 2021, 36, 115-122.	18.0	23
120	High voltage and robust lithium metal battery enabled by highly-fluorinated interphases. <i>Energy Storage Materials</i> , 2022, 51, 317-326.	18.0	22
121	Temperature Dependence of Carbon-13 Kinetic Isotope Effects of Importance to Global Climate Change. <i>Journal of the American Chemical Society</i> , 2005, 127, 2830-2831.	13.7	21
122	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.	10.3	21
123	Transition metals doped borophene-graphene heterostructure for robust polysulfide anchoring: A first principle study. <i>Applied Surface Science</i> , 2020, 534, 147575.	6.1	18
124	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.	10.3	18
125	Exploring the anchoring effect and catalytic mechanism of 3d transition metal phthalocyanine for S ₈ /LiPSs: A density functional theory study. <i>Applied Surface Science</i> , 2021, 558, 149928.	6.1	17
126	Theoretical study on mechanism for O ₃ -initiated atmospheric oxidation reaction of β -caryophyllene. <i>Computational and Theoretical Chemistry</i> , 2010, 947, 68-75.	1.5	16

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127	Computational investigation of 2D 3d/4d hexagonal transition metal borides for metal-ion batteries. <i>Electrochimica Acta</i> , 2021, 384, 138404.	5.2	16
128	Atomistic Modeling of PEDOT:PSS Complexes I: DFT Benchmarking. <i>Macromolecules</i> , 2021, 54, 3634-3646.	4.8	14
129	Suppressing Polysulfide Shuttling in Lithium-Sulfur Batteries via a Multifunctional Conductive Binder. <i>Small Methods</i> , 2021, 5, e2100839.	8.6	14
130	The OH-initiated chemical transformation of 1,2,4,6,8,10,11-heptachloroundecane in the atmosphere. <i>RSC Advances</i> , 2015, 5, 37988-37994.	3.6	13
131	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.	12.9	13
132	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.	5.0	13
133	The nature of the π - π interactions and a comparative study with the nature of the π - π interactions. <i>Computational and Theoretical Chemistry</i> , 2014, 1030, 1-8.	2.5	10
134	Stereospecific Synthesis of Fluorinated Pyrazolidinones and Isoxazolidines via a Catalyst-Free 1,3-Dipolar Cycloaddition of β -Fluoroalkylated α,β -Unsaturated α -Pyridylsulfones. <i>Asian Journal of Organic Chemistry</i> , 2018, 7, 1830-1834.		10
135	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.	2.0	10
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