Yan Zhao

List of Publications by Year
in descending order

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		11608	5965
160	65,889	70	160
papers	citations	h-index	g-index

163	163	163	40123
all docs	docs citations	times ranked	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. Theoretical Chemistry Accounts, 2008, 120, 215-241.	0.5	23,928
2	Density Functionals with Broad Applicability in Chemistry. Accounts of Chemical Research, 2008, 41, 157-167.	7.6	6,193
3	A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions. Journal of Chemical Physics, 2006, 125, 194101.	1.2	4,175
4	Design of Density Functionals by Combining the Method of Constraint Satisfaction with Parametrization for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2006, 2, 364-382.	2.3	3,329
5	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
6	Hybrid Meta Density Functional Theory Methods for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions:â€‰ The MPW1B95 and MPWB1K Models and Comparative Assessments for Hydrogen Bonding and van der Waals Interactions. Journal of Physical Chemistry A, 2004, 108, 6908-6918.	1.1	1,497
7	Design of Density Functionals That Are Broadly Accurate for Thermochemistry, Thermochemical Kinetics, and Nonbonded Interactions. Journal of Physical Chemistry A, 2005, 109, 5656-5667.	1.1	1,451
8	Computational Thermochemistry: Scale Factor Databases and Scale Factors for Vibrational Frequencies Obtained from Electronic Model Chemistries. Journal of Chemical Theory and Computation, 2010, 6, 2872-2887.	2.3	1,183
9	Density Functional for Spectroscopy:Â No Long-Range Self-Interaction Error, Good Performance for Rydberg and Charge-Transfer States, and Better Performance on Average than B3LYP for Ground States. Journal of Physical Chemistry A, 2006, 110, 13126-13130.	1.1	1,140
10	Exchange-correlation functional with broad accuracy for metallic and nonmetallic compounds, kinetics, and noncovalent interactions. Journal of Chemical Physics, 2005, 123, 161103.	1.2	979
11	Exploring the Limit of Accuracy of the Global Hybrid Meta Density Functional for Main-Group Thermochemistry, Kinetics, and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2008, 4, 1849-1868.	2.3	956
12	Twinborn TiO₂â€“TiN heterostructures enabling smooth trappingâ€“diffusionâ€“conversion of polysulfides towards ultralong life lithiumâ€“sulfur batteries. Energy and Environmental Science, 2017, 10, 1694-1703.	15.6	884
13	Benchmark Databases for Nonbonded Interactions and Their Use To Test Density Functional Theory. Journal of Chemical Theory and Computation, 2005, 1, 415-432.	2.3	832
14	Benchmark Database of Barrier Heights for Heavy Atom Transfer, Nucleophilic Substitution, Association, and Unimolecular Reactions and Its Use to Test Theoretical Methods. Journal of Physical Chemistry A, 2005, 109, 2012-2018.	1.1	736
15	Comparative DFT Study of van der Waals Complexes:Â Rare-Gas Dimers, Alkaline-Earth Dimers, Zinc Dimer, and Zinc-Rare-Gas Dimers. Journal of Physical Chemistry A, 2006, 110, 5121-5129.	1.1	706
16	Effectiveness of Diffuse Basis Functions for Calculating Relative Energies by Density Functional Theory. Journal of Physical Chemistry A, 2003, 107, 1384-1388.	1.1	688
17	Applications and validations of the Minnesota density functionals. Chemical Physics Letters, 2011, 502, 1-13.	1.2	662
18	Development and Assessment of a New Hybrid Density Functional Model for Thermochemical Kinetics. Journal of Physical Chemistry A, 2004, 108, 2715-2719.	1.1	639

#	ARTICLE	IF	CITATIONS
19	Density Functionals for Noncovalent Interaction Energies of Biological Importance. Journal of Chemical Theory and Computation, 2007, 3, 289-300.	2.3	557
20	The DBH24/08 Database and Its Use to Assess Electronic Structure Model Chemistries for Chemical Reaction Barrier Heights. Journal of Chemical Theory and Computation, 2009, 5, 808-821.	2.3	462
21	Density Functionals for Inorganometallic and Organometallic Chemistry. Journal of Physical Chemistry A, 2005, 109, 11127-11143.	1.1	447
22	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	1.2	425
23	Multi-coefficient extrapolated density functional theory for thermochemistry and thermochemical kinetics. Physical Chemistry Chemical Physics, 2005, 7, 43.	1.3	393
24	On the Performances of the M06 Family of Density Functionals for Electronic Excitation Energies. Journal of Chemical Theory and Computation, 2010, 6, 2071-2085.	2.3	383
25	How Well Can New-Generation Density Functionals Describe the Energetics of Bond-Dissociation Reactions Producing Radicals?. Journal of Physical Chemistry A, 2008, 112, 1095-1099.	1.1	359
26	Lithiophilic-lithiophobic gradient interfacial layer for a highly stable lithium metal anode. Nature Communications, 2018, 9, 3729.	5.8	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. Journal of Chemical Theory and Computation, 2009, 5, 324-333.	2.3	313
28	Doubly Hybrid Meta DFT:â€‰ New Multi-Coefficient Correlation and Density Functional Methods for Thermochemistry and Thermochemical Kinetics. Journal of Physical Chemistry A, 2004, 108, 4786-4791.	1.1	297
29	Construction of a generalized gradient approximation by restoring the density-gradient expansion and enforcing a tight Liebâ€“Oxford bound. Journal of Chemical Physics, 2008, 128, 184109.	1.2	260
30	A 3D Nitrogenâ€Doped Graphene/TiN Nanowires Composite as a Strong Polysulfide Anchor for Lithiumâ€“Sulfur Batteries with Enhanced Rate Performance and High Areal Capacity. Advanced Materials, 2018, 30, e1804089.	11.1	251
31	Ru-doped 3D flower-like bimetallic phosphide with a climbing effect on overall water splitting. Applied Catalysis B: Environmental, 2020, 279, 119396.	10.8	251
32	How well can new-generation density functional methods describe stacking interactions in biological systems?. Physical Chemistry Chemical Physics, 2005, 7, 2701.	1.3	246
33	Tests of second-generation and third-generation density functionals for thermochemical kineticsElectronic supplementary information (ESI) available: Mean errors for pure and hybrid DFT methods. See http://www.rsc.org/suppdata/cp/b3/b316260e/. Physical Chemistry Chemical Physics, 2004, 6, 673.	1.3	242
34	Computational characterization and modeling of buckyball tweezers: density functional study of concaveâ€“convex Ï€â‹¯Ï€ interactions. Physical Chemistry Chemical Physics, 2008, 10, 2813.	1.3	218
35	Assessment of Model Chemistries for Noncovalent Interactions. Journal of Chemical Theory and Computation, 2006, 2, 1009-1018.	2.3	214
36	Databases for Transition Element Bonding:Â Metalâ^'Metal Bond Energies and Bond Lengths and Their Use To Test Hybrid, Hybrid Meta, and Meta Density Functionals and Generalized Gradient Approximations. Journal of Physical Chemistry A, 2005, 109, 4388-4403.	1.1	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. Journal of Chemical Theory and Computation, 2007, 3, 569-582.	2.3	207
38	Tests of the RPBE, revPBE, Ï„-HCTHhyb, Ï‰B97X-D, and MOHLYP density functional approximations and 29 others against representative databases for diverse bond energies and barrier heights in catalysis. Journal of Chemical Physics, 2010, 132, 164117.	1.2	206
39	Lowâ€Bandgap Seâ€Deficient Antimony Selenide as a Multifunctional Polysulfide Barrier toward Highâ€Performance Lithiumâ€“Sulfur Batteries. Advanced Materials, 2020, 32, e1904876.	11.1	206
40	Assessment of Density Functionals for Ï€ Systems:Â Energy Differences between Cumulenes and Poly-ynes; Proton Affinities, Bond Length Alternation, and Torsional Potentials of Conjugated Polyenes; and Proton Affinities of Conjugated Shiff Bases. Journal of Physical Chemistry A, 2006, 110, 10478-10486.	1.1	196
41	Multilayer stabilization for fabricating high-loading single-atom catalysts. Nature Communications, 2020, 11, 5892.	5.8	195
42	A Density Functional That Accounts for Medium-Range Correlation Energies in Organic Chemistry. Organic Letters, 2006, 8, 5753-5755.	2.4	193
43	Density Functional Theory for Reaction Energies: Test of Meta and Hybrid Meta Functionals, Range-Separated Functionals, and Other High-Performance Functionals. Journal of Chemical Theory and Computation, 2011, 7, 669-676.	2.3	190
44	Density Functional Theory for Battery Materials. Energy and Environmental Materials, 2019, 2, 264-279.	7.3	186
45	Comparative assessment of density functional methods for 3d transition-metal chemistry. Journal of Chemical Physics, 2006, 124, 224105.	1.2	180
46	Strain Engineering of a MXene/CNT Hierarchical Porous Hollow Microsphere Electrocatalyst for a Highâ€Efficiency Lithium Polysulfide Conversion Process. Angewandte Chemie - International Edition, 2021, 60, 2371-2378.	7.2	176
47	Generalized Gradient Approximation That Recovers the Second-Order Density-Gradient Expansion with Optimized Across-the-Board Performance. Journal of Physical Chemistry Letters, 2011, 2, 1991-1997.	2.1	171
48	How Well Can Density Functional Methods Describe Hydrogen Bonds to Ï€ Acceptors?. Journal of Physical Chemistry B, 2005, 109, 19046-19051.	1.2	169
49	Attractive Noncovalent Interactions in the Mechanism of Grubbs Second-Generation Ru Catalysts for Olefin Metathesis. Organic Letters, 2007, 9, 1967-1970.	2.4	163
50	Identification of Phase Control of Carbonâ€Confined Nb₂O₅ Nanoparticles toward Highâ€Performance Lithium Storage. Advanced Energy Materials, 2019, 9, 1802695.	10.2	161
51	Benchmark Data for Interactions in Zeolite Model Complexes and Their Use for Assessment and Validation of Electronic Structure Methods. Journal of Physical Chemistry C, 2008, 112, 6860-6868.	1.5	157
52	A Prototype for Graphene Material Simulation:â€‰ Structures and Interaction Potentials of Coronene Dimers. Journal of Physical Chemistry C, 2008, 112, 4061-4067.	1.5	152
53	High-Voltage Cycling Induced Thermal Vulnerability in LiCoO₂ Cathode: Cation Loss and Oxygen Release Driven by Oxygen Vacancy Migration. ACS Nano, 2020, 14, 6181-6190.	7.3	144
54	The 6-31B(d) Basis Set and the BMC-QCISD and BMC-CCSD Multicoefficient Correlation Methods. Journal of Physical Chemistry A, 2005, 109, 1643-1649.	1.1	138

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55	Verdict: Time-Dependent Density Functional Theory â€œNot Guiltyâ€•of Large Errors for Cyanines. Journal of Chemical Theory and Computation, 2012, 8, 1255-1259.	2.3	122
56	Thermochemical Kinetics for Multireference Systems: Addition Reactions of Ozone. Journal of Physical Chemistry A, 2009, 113, 5786-5799.	1.1	114
57	Quicker and More Zn²⁺ Storage Predominantly from the Interface. Advanced Materials, 2021, 33, e2100359.	11.1	111
58	Significant Improvements in Dielectric Constant and Energy Density of Ferroelectric Polymer Nanocomposites Enabled by Ultralow Contents of Nanofillers. Advanced Materials, 2021, 33, e2102392.	11.1	102
59	Multicoefficient Extrapolated Density Functional Theory Studies of Ï€Â·Â·Â·Ï€ Interactions:Â The Benzene Dimer. Journal of Physical Chemistry A, 2005, 109, 4209-4212.	1.1	99
60	Density Functional Theory for Electrocatalysis. Energy and Environmental Materials, 2022, 5, 157-185.	7.3	95
61	Coordinatively Deficient Single-atom Fe-N-C Electrocatalyst with Optimized Electronic Structure for High-performance Lithium-sulfur Batteries. Energy Storage Materials, 2022, 46, 269-277.	9.5	95
62	Improved Description of Nuclear Magnetic Resonance Chemical Shielding Constants Using the M06-L Meta-Generalized-Gradient-Approximation Density Functional. Journal of Physical Chemistry A, 2008, 112, 6794-6799.	1.1	92
63	Allâ€Purpose Electrode Design of Flexible Conductive Scaffold toward Highâ€Performance Liâ€“S Batteries. Advanced Functional Materials, 2020, 30, 2000613.	7.8	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. Journal of Physical Chemistry A, 2005, 109, 6624-6627.	1.1	89
65	Size-Selective Supramolecular Chemistry in a Hydrocarbon Nanoring. Journal of the American Chemical Society, 2007, 129, 8440-8442.	6.6	89
66	Metalâ€Organic Frameworks Nanocomposites with Different Dimensionalities for Energy Conversion and Storage. Advanced Energy Materials, 2022, 12, 2100346.	10.2	86
67	A robust electrospun separator modified with in situ grown metal-organic frameworks for lithium-sulfur batteries. Chemical Engineering Journal, 2020, 395, 124979.	6.6	85
68	Validation of electronic structure methods for isomerization reactions of large organic molecules. Physical Chemistry Chemical Physics, 2011, 13, 13683.	1.3	78
69	Calculation of semiconductor band gaps with the M06-L density functional. Journal of Chemical Physics, 2009, 130, 074103.	1.2	75
70	Construction of Oxygen-Deficient La(OH)₃ Nanorods Wrapped by Reduced Graphene Oxide for Polysulfide Trapping toward High-Performance Lithium/Sulfur Batteries. ACS Applied Materials & Interfaces, 2019, 11, 23271-23279.	4.0	71
71	Revealing the atomistic origin of the disorder-enhanced Na-storage performance in NaFePO4 battery cathode. Nano Energy, 2019, 57, 608-615.	8.2	67
72	Facile formation of tetragonal-Nb2O5 microspheres for high-rate and stable lithium storage with high areal capacity. Science Bulletin, 2020, 65, 1154-1162.	4.3	64

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73	Improved CO Adsorption Energies, Site Preferences, and Surface Formation Energies from a Meta-Generalized Gradient Approximation Exchangeâ€“Correlation Functional, M06-L. Journal of Physical Chemistry Letters, 2012, 3, 2975-2979.	2.1	63
74	Benchmark Database for Ylidic Bond Dissociation Energies and Its Use for Assessments of Electronic Structure Methods. Journal of Chemical Theory and Computation, 2012, 8, 2824-2834.	2.3	62
75	Benchmarking approximate density functional theory for s/d excitation energies in 3d transition metal cations. Journal of Computational Chemistry, 2008, 29, 185-189.	1.5	61
76	Thermochemical Kinetics of Hydrogen-Atom Transfers between Methyl, Methane, Ethynyl, Ethyne, and Hydrogen. Journal of Physical Chemistry A, 2007, 111, 4632-4642.	1.1	59
77	Carbene Rotamer Switching Explains the Reverse Trans Effect in Forming the Grubbs Second-Generation Olefin Metathesis Catalyst. Organometallics, 2011, 30, 4196-4200.	1.1	59
78	Interface enhanced well-dispersed Co9S8 nanocrystals as an efficient polysulfide host in lithiumâ€“sulfur batteries. Journal of Energy Chemistry, 2020, 48, 109-115.	7.1	59
79	Coordination environments tune the activity of oxygen catalysis on single atom catalysts: A computational study. Nano Research, 2022, 15, 3073-3081.	5.8	58
80	Highly active Fe centered FeM-N-doped carbon (MÂ=ÂCo/Ni/Mn): A general strategy for efficient oxygen conversion in Znâ€“air battery. Chemical Engineering Journal, 2021, 424, 130559.	6.6	55
81	Significantly enhancing the dielectric constant and breakdown strength of linear dielectric polymers by utilizing ultralow loadings of nanofillers. Journal of Materials Chemistry A, 2021, 9, 23028-23036.	5.2	54
82	Tunable <scp>Ruâ€Ru₂P</scp> heterostructures with charge redistribution for efficient <scp>pHâ€universal</scp> hydrogen evolution. InformaÄnÃ-MateriÃ¡ly, 2022, 4, .	8.5	53
83	High Yield Electrosynthesis of Hydrogen Peroxide from Water Using Electrospun CaSnO₃@Carbon Fiber Membrane Catalysts with Abundant Oxygen Vacancy. Advanced Functional Materials, 2021, 31, 2100099.	7.8	52
84	Development of a curcumin-based antifouling and anticorrosion sustainable polybenzoxazine resin composite coating. Composites Part B: Engineering, 2021, 225, 109263.	5.9	51
85	Binding energy of d10 transition metals to alkenes by wave function theory and density functional theoryâ˜†. Journal of Molecular Catalysis A, 2010, 324, 80-88.	4.8	50
86	Gradient SEI layer induced by liquid alloy electrolyte additive for high rate lithium metal battery. Nano Energy, 2021, 88, 106237.	8.2	48
87	Combined valence bond-molecular mechanics potential-energy surface and direct dynamics study of rate constants and kinetic isotope effects for the H+C2H6 reaction. Journal of Chemical Physics, 2006, 124, 044315.	1.2	47
88	Density Functional Calculations of E2 and S_N2 Reactions: Effects of the Choice of Density Functional, Basis Set, and Self-Consistent Iterations. Journal of Chemical Theory and Computation, 2010, 6, 1104-1108.	2.3	45
89	Nanoâ€Ferric Oxide Embedded in Graphene Oxide: Highâ€performance Electrocatalyst for Nitrogen Reduction at Ambient Condition. Energy and Environmental Materials, 2021, 4, 88-94.	7.3	44
90	Diastereodivergent Asymmetric 1,3â€Dipolar Cycloaddition of Azomethine Ylides and Î²â€Fluoroalkyl Vinylsulfones: Low Copper(II) Catalyst Loading and Theoretical Studies. Angewandte Chemie - International Edition, 2019, 58, 16637-16643.	7.2	43

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91	Three-dimensional porous N-doped graphitic carbon framework with embedded CoO for photocatalytic CO2 reduction. Applied Catalysis B: Environmental, 2021, 298, 120546.	10.8	42
92	Bioinspired mechanically interlocking holey graphene@SiO₂ anode. , 2022, 1, 517-525.		42
93	How Well Can New-Generation Density Functionals Describe Protonated Epoxides Where Older Functionals Fail?. Journal of Organic Chemistry, 2007, 72, 295-298.	1.7	41
94	Effect of Triton X-100 on the stability of aqueous dispersions of copper phthalocyanine pigment nanoparticles. Journal of Colloid and Interface Science, 2011, 362, 33-41.	5.0	40
95	Facilitating the acidic oxygen reduction of Feâ€“Nâ€“C catalysts by fluorine-doping. Materials Horizons, 2022, 9, 417-424.	6.4	39
96	Multiconfiguration Molecular Mechanics Based on Combined Quantum Mechanical and Molecular Mechanical Calculations. Journal of Chemical Theory and Computation, 2006, 2, 1237-1254.	2.3	38
97	â€œSoft on rigidâ€•nanohybrid as the self-supporting multifunctional cathode electrocatalyst for high-performance lithium-polysulfide batteries. Nano Energy, 2020, 78, 105293.	8.2	36
98	Oxygen defects boost polysulfides immobilization and catalytic conversion: First-principles computational characterization and experimental design. Nano Research, 2020, 13, 2299-2307.	5.8	36
99	Three-Dimensional Porous Nitrogen-Doped Carbon Nanosheet with Embedded Ni_xCo_{3â€“x}S₄ Nanocrystals for Advanced Lithiumâ€“Sulfur Batteries. ACS Applied Materials & Interfaces, 2020, 12, 9181-9189.	4.0	36
100	Gradient sulfur fixing separator with catalytic ability for stable lithium sulfur battery. Chemical Engineering Journal, 2021, 422, 130107.	6.6	36
101	Virtual screening of two-dimensional selenides and transition metal doped SnSe for lithium-sulfur batteries: A first-principles study. Applied Surface Science, 2021, 570, 151213.	3.1	36
102	Electronic Regulation of ZnCo Dualâ€Atomic Active Sites Entrapped in 1D@2D Hierarchical Nâ€Doped Carbon for Efficient Synergistic Catalysis of Oxygen Reduction in Znâ€“Air Battery. Small, 2022, 18, e2107141.	5.2	36
103	Low-coordinated cobalt arrays for efficient hydrazine electrooxidation. Energy and Environmental Science, 2022, 15, 3246-3256.	15.6	36
104	The Minnesota Density Functionals and their Applications to Problems in Mineralogy and Geochemistry. Reviews in Mineralogy and Geochemistry, 2010, 71, 19-37.	2.2	35
105	Computational Design of Single Mo Atom Anchored Defective Boron Phosphide Monolayer as a Highâ€performance Electrocatalyst for the Nitrogen Reduction Reaction. Energy and Environmental Materials, 2021, 4, 255-262.	7.3	35
106	Extrapolation of high-order correlation energies: the WMS model. Physical Chemistry Chemical Physics, 2018, 20, 27375-27384.	1.3	34
107	Accurate Binding Energies for Lithium Polysulfides and Assessment of Density Functionals for Lithiumâ€“Sulfur Battery Research. Journal of Physical Chemistry C, 2019, 123, 20737-20747.	1.5	34
108	Uniform zeolitic imidazolate framework coating via in situ recoordination for efficient polysulfide trapping. Energy Storage Materials, 2019, 23, 55-61.	9.5	33

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109	Atomic-Level Modulation of the Interface Chemistry of Platinumâ€“Nickel Oxide toward Enhanced Hydrogen Electrocatalysis Kinetics. Nano Letters, 2021, 21, 4845-4852.	4.5	31
110	Multicoefficient Gaussian-3 Calculation of the Rate Constant for the OH + CH4Reaction and Its12C/13C Kinetic Isotope Effect with Emphasis on the Effects of Coordinate System and Torsional Treatment. Journal of Physical Chemistry A, 2007, 111, 11706-11717.	1.1	30
111	Benchmark Data for Noncovalent Interactions in HCOOHÂ·Â·Â·Benzene Complexes and Their Use for Validation of Density Functionals. Journal of Chemical Theory and Computation, 2009, 5, 2726-2733.	2.3	30
112	A three-dimensional nitrogen-doped graphene framework decorated with an atomic layer deposited ultrathin V₂O₅ layer for lithium sulfur batteries with high sulfur loading. Journal of Materials Chemistry A, 2020, 8, 12106-12113.	5.2	28
113	Establishing a theoretical insight for penta-coordinated iron-nitrogen-carbon catalysts toward oxygen reaction. Nano Research, 2022, 15, 6067-6075.	5.8	28
114	Trimetallic Sulfide Hollow Superstructures with Engineered dâ€Band Center for Oxygen Reduction to Hydrogen Peroxide in Alkaline Solution. Advanced Science, 2022, 9, e2104768.	5.6	26
115	Polymer dielectrics exhibiting an anomalously improved dielectric constant simultaneously achieved high energy density and efficiency enabled by CdSe/Cd_{1â^'x}Zn_xS quantum dots. Journal of Materials Chemistry A, 2020, 8, 13659-13670.	5.2	25
116	Theoretical insights into dual-atom catalysts for the oxygen reduction reaction: the crucial role of orbital polarization. Journal of Materials Chemistry A, 2022, 10, 9150-9160.	5.2	25
117	Comment on â€œMore accurate generalized gradient approximation for solidsâ€• Physical Review B, 2008, 78, .	1.1	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. Langmuir, 2010, 26, 6995-7006.	1.6	23
119	Interface cation migration kinetics induced oxygen release heterogeneity in layered lithium cathodes. Energy Storage Materials, 2021, 36, 115-122.	9.5	23
120	High voltage and robust lithium metal battery enabled by highly-fluorinated interphases. Energy Storage Materials, 2022, 51, 317-326.	9.5	22
121	Temperature Dependence of Carbon-13 Kinetic Isotope Effects of Importance to Global Climate Change. Journal of the American Chemical Society, 2005, 127, 2830-2831.	6.6	21
122	Novel graphitic carbon nitride g-C₉N₁₀ as a promising platform to design efficient photocatalysts for dinitrogen reduction to ammonia: the first-principles investigation. Journal of Materials Chemistry A, 2021, 9, 20615-20625.	5.2	21
123	Transition metals doped borophene-graphene heterostructure for robust polysulfide anchoring: A first principle study. Applied Surface Science, 2020, 534, 147575.	3.1	18
124	Coreâ€“shell Cu@Cu₂O nanoparticles embedded in 3D honeycomb-like N-doped graphitic carbon for photocatalytic CO₂ reduction. Journal of Materials Chemistry A, 2022, 10, 4758-4769.	5.2	18
125	Exploring the anchoring effect and catalytic mechanism of 3d transition metal phthalocyanine for S8/LiPSs: A density functional theory study. Applied Surface Science, 2021, 558, 149928.	3.1	17
126	Theoretical study on mechanism for O3-initiated atmospheric oxidation reaction of Î²-caryophyllene. Computational and Theoretical Chemistry, 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. Electrochimica Acta, 2021, 384, 138404.	2.6	16
128	Atomistic Modeling of PEDOT:PSS Complexes I: DFT Benchmarking. Macromolecules, 2021, 54, 3634-3646.	2.2	14
129	Suppressing Polysulfide Shuttling in Lithiumâ€“Sulfur Batteries via a Multifunctional Conductive Binder. Small Methods, 2021, 5, e2100839.	4.6	14
130	The OH-initiated chemical transformation of 1,2,4,6,8,10,11-heptachloroundecane in the atmosphere. RSC Advances, 2015, 5, 37988-37994.	1.7	13
131	Structural properties and electrochemical performance of different polymorphs of Nb2O5 in magnesium-based batteries. Journal of Energy Chemistry, 2021, 58, 586-592.	7.1	13
132	Znâ€“Co Zeolitic Imidazolate Framework Nanoparticles Intercalated in Graphene Nanosheets for Room-Temperature NO₂ Sensing. ACS Applied Nano Materials, 2021, 4, 3998-4006.	2.4	13
133	The nature of the Iâ‹¯I interactions and a comparative study with the nature of the Ï€â‹¯Ï€ interactions. Computational and Theoretical Chemistry, 2014, 1030, 1-8.	1.1	10
134	Stereospecific Synthesis of Fluorinated Pyrazolidinones and Isoxazolidines via a Catalystâ€Free 1,3â€Dipolar Cycloaddition of Î²â€Fluoroalkylated Î±,Î²â€Unsaturated 2â€Pyridylsulfones. Asian Journal of Organic Chemistry, 2018, 7, 1830-1834.	1.3	10
135	Diastereodivergent Asymmetric 1,3â€Dipolar Cycloaddition of Azomethine Ylides and Î²â€Fluoroalkyl Vinylsulfones: Low Copper(II) Catalyst Loading and Theoretical Studies. Angewandte Chemie, 2019, 131, 16790-16796.	1.6	10
136	Novel Two-Dimensional Metal-Based Ï€-d Conjugated Nanosheets as Photocatalyst for Nitrogen Reduction Reaction: The First-Principle Investigation. ACS Applied Materials & Interfaces, 2022, 14, 5384-5394.	4.0	10
137	Adsorption of Myrj 45 on copper phthalocyanine pigment nanoparticles and effect on their dispersion stability in aqueous solution. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2011, 390, 74-85.	2.3	9
138	Theoretical study on the reaction mechanism of vinyl acetate with OH radicals in the atmosphere. Canadian Journal of Chemistry, 2013, 91, 241-247.	0.6	9
139	Atomistic Modeling of PEDOT:PSS Complexes II: Force Field Parameterization. Macromolecules, 2021, 54, 5354-5365.	2.2	9
140	Accelerating conversion of LiPSs on strain-induced MXene for high-performance Li-S battery. Chemical Engineering Journal, 2022, 439, 135679.	6.6	9
141	Computation of Nonretarded London Dispersion Coefficients and Hamaker Constants of Copper Phthalocyanine. Journal of Chemical Theory and Computation, 2010, 6, 491-498.	2.3	8
142	â€˜Be waterâ€™ strategy of liquid lithium sulfide enables 0.2ÂV potential barrier for high-performance lithiumâ€“sulfur batteries. Materials Today Energy, 2021, 21, 100793.	2.5	8
143	A facile surface alloy-engineering route to enable robust lithium metal anodes. Physical Chemistry Chemical Physics, 2022, 24, 4751-4758.	1.3	8
144	Stereoconvergent and stepwise 1,3-dipolar cycloadditions of nitrile oxides and nitrile imines. Chinese Chemical Letters, 2022, 33, 3012-3016.	4.8	8

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145	Revealing the Multiâ€Electron Reaction Mechanism of Na₃V₂O₂(PO₄)₂F Towards Improved Lithium Storage. ChemSusChem, 2021, 14, 2984-2991.	3.6	6
146	Accurate redox potentials for solvents in <scp>Liâ€metal</scp> batteries and assessment of density functionals. International Journal of Quantum Chemistry, 2022, 122, .	1.0	6
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