

Baoshan Wang

List of Publications by Year in descending order

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60
papers

2,675
citations

361413

20
h-index

197818

49
g-index

60
all docs

60
docs citations

60
times ranked

3231
citing authors

#	ARTICLE	IF	CITATIONS
1	A Pyrene-Based, Fluorescent Three-Dimensional Covalent Organic Framework. <i>Journal of the American Chemical Society</i> , 2016, 138, 3302-3305.	13.7	628
2	3D Porphyrin-Based Covalent Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2017, 139, 8705-8709.	13.7	369
3	An AI-Egen-based 3D covalent organic framework for white light-emitting diodes. <i>Nature Communications</i> , 2018, 9, 5234.	12.8	293
4	A 2D porous porphyrin-based covalent organic framework for sulfur storage in lithium-sulfur batteries. <i>Journal of Materials Chemistry A</i> , 2016, 4, 7416-7421.	10.3	267
5	A Tetrathiafulvalene-Based Electroactive Covalent Organic Framework. <i>Chemistry - A European Journal</i> , 2014, 20, 14614-14618.	3.3	143
6	Fractal Analysis on Pore Structure and Hydration of Magnesium Oxysulfate Cements by First Principle, Thermodynamic and Microstructure-Based Methods. <i>Fractal and Fractional</i> , 2021, 5, 164.	3.3	111
7	Ab initio study of the reaction of propionyl (C ₂ H ₅ CO) radical with oxygen (O ₂). <i>Journal of Chemical Physics</i> , 2007, 127, 054306.	3.0	61
8	Surface Sensitive Photoluminescence of Carbon Nanodots: Coupling between the Carbonyl Group and π -Electron System. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3621-3629.	4.6	61
9	A Systematic Computational Study on the Reactions of HO ₂ with RO ₂ : The HO ₂ + CH ₃ O ₂ (CD ₃ O ₂) and HO ₂ + CH ₂ FO ₂ Reactions. <i>Journal of Physical Chemistry A</i> , 2005, 109, 451-460.	2.5	56
10	An improved B3LYP method in the calculation of organic thermochemistry and reactivity. <i>Computational and Theoretical Chemistry</i> , 2013, 1015, 64-71.	2.5	56
11	Extensive theoretical studies of a new energetic material: Tetrazino-tetrazine-tetraoxide (TTTO). <i>Journal of Computational Chemistry</i> , 2009, 30, 1816-1820.	3.3	55
12	Theoretical investigations on the SO ₂ +HO ₂ reaction and the SO ₂ -HO ₂ radical complex. <i>Chemical Physics Letters</i> , 2005, 410, 235-241.	2.6	48
13	Prediction on dielectric strength and boiling point of gaseous molecules for replacement of SF ₆ . <i>Journal of Computational Chemistry</i> , 2017, 38, 721-729.	3.3	47
14	A Systematic Computational Study of the Reactions of HO ₂ with RO ₂ : The HO ₂ + CH ₂ ClO ₂ , CHCl ₂ O ₂ , and CCl ₃ O ₂ Reactions. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9299-9309.	2.5	38
15	Mechanistic and kinetic study of the CH ₃ CO+O ₂ reaction. <i>Journal of Chemical Physics</i> , 2005, 122, 224304.	3.0	34
16	A Systematic Computational Study of the Reactions of HO ₂ with RO ₂ : The HO ₂ + C ₂ H ₅ O ₂ Reaction. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11206-11212.	2.5	31
17	Mechanistic and Kinetic Investigations on the Thermal Unimolecular Reaction of Heptafluoroisobutyronitrile. <i>Journal of Physical Chemistry A</i> , 2018, 122, 7704-7715.	2.5	31
18	Insulation condition monitoring of epoxy spacers in GIS using a decomposed gas CS ₂ . <i>IEEE Transactions on Dielectrics and Electrical Insulation</i> , 2013, 20, 2152-2157.	2.9	24

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19	Theoretical Study of the Adsorption/Dissociation Reactions of Formic Acid on the $\text{Al}_2\text{O}_3(0001)$ Surface. <i>Journal of Physical Chemistry C</i> , 2014, 118, 20889-20898.	3.1	23
20	Synthesis and Dielectric Properties of Trifluoromethanesulfonyl Fluoride: An Alternative Gas to SF_6 . <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 21913-21920.	3.7	21
21	Facile Synthesis of Polyphenothiazine as a High-Performance pH -Type Cathode for Rechargeable Lithium Batteries. <i>ChemSusChem</i> , 2021, 14, 3174-3181.	6.8	21
22	Mechanisms of Modulation of Calcium Phosphate Pathological Mineralization by Mobile and Immobile Small-Molecule Inhibitors. <i>Journal of Physical Chemistry B</i> , 2018, 122, 1580-1587.	2.6	20
23	Detection of intense partial discharge of epoxy insulation in SF_6 insulated equipment using carbonyl sulfide. <i>IEEE Transactions on Dielectrics and Electrical Insulation</i> , 2016, 23, 2942-2948.	2.9	19
24	<i>A Priori</i> Theoretical Model for Discovery of Environmentally Sustainable Perfluorinated Compounds. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3462-3469.	2.5	18
25	Preparation of Monodisperse Hydrophilic Quantum Dots with Amphiphilic Polymers. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 39901-39906.	8.0	17
26	Role of Alcoholic Hydroxyls of Dicarboxylic Acids in Regulating Nanoscale Dissolution Kinetics of Dicalcium Phosphate Dihydrate. <i>ACS Sustainable Chemistry and Engineering</i> , 2017, 5, 3920-3928.	6.7	16
27	Covalent Organic Frameworks for Simultaneous CO_2 Capture and Selective Catalytic Transformation. <i>Catalysts</i> , 2021, 11, 1133.	3.5	16
28	Dielectric Properties of $\text{CF}_3\text{SO}_2\text{F}/\text{N}_2$ and $\text{CF}_3\text{SO}_2\text{F}/\text{CO}_2$ Mixtures as a Substitute to SF_6 . <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 15796-15804.	3.7	15
29	High-Performance Polymeric Lithium Salt Electrode Material from Phenol-Formaldehyde Condensation. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 37289-37298.	8.0	15
30	Development and application of a ReaxFF reactive force field for molecular dynamics of perfluorinated ketones thermal decomposition. <i>Chemical Physics</i> , 2020, 538, 110888.	1.9	14
31	Theoretical study of the mechanisms and kinetics of the reactions of hydroperoxy (HO_2) radicals with hydroxymethylperoxy (HOCH_2O_2) and methoxymethylperoxy ($\text{CH}_3\text{OCH}_2\text{O}_2$) radicals. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 22805-22814.	2.8	12
32	Experimental and Theoretical Study on the OH-Reaction Kinetics and Photochemistry of Acetyl Fluoride ($\text{CH}_3\text{C}(\text{O})\text{F}$), an Atmospheric Degradation Intermediate of HFC-161 ($\text{C}_2\text{H}_5\text{F}$). <i>Journal of Physical Chemistry A</i> , 2015, 119, 7753-7765.	2.5	10
33	Phosphoric acid functionalized magnetic sorbents for selective enrichment of TiO_2 nanoparticles in surface water followed by inductively coupled plasma mass spectrometry detection. <i>Science of the Total Environment</i> , 2020, 703, 135464.	8.0	9
34	Atmospheric Chemistry of Perfluoro-3-methyl-2-butanone [$\text{CF}_3\text{C}(\text{O})\text{CF}(\text{CF}_3)_2$]: Photodissociation and Reaction with OH Radicals. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8840-8848.	2.5	8
35	Computational Study of the Ion-Molecule Reactions Involving Fluxional Cations: CH_4^{++} , H_2^+ , CH_5^{++} , H and Isotope Effect. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8537-8547.	2.5	7
36	Double-Layered Composite Methods Extrapolating to Complete Basis-Set Limit for the Systems Involving More than Ten Heavy Atoms: Application to the Reaction of Heptafluoroisobutyronitrile with Hydroxyl Radical. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9020-9032.	2.5	7

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37	Theoretical study of the hydrolysis of sulfur tetrafluoride. <i>Journal of Fluorine Chemistry</i> , 2013, 153, 114-120.	1.7	6
38	Theoretical Investigations on the Oxidation of Heptafluoro-iso-butyronitrile by Atomic Oxygen in Dielectric Breakdown. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8398-8413.	2.5	6
39	ReaxFF reactive force field development and application for molecular dynamics simulations of heptafluoroisobutyronitrile thermal decomposition. <i>Chemical Physics Letters</i> , 2020, 751, 137554.	2.6	6
40	6-Iodopurine as a Versatile Building Block for RNA Purine Architecture Modifications. <i>Bioconjugate Chemistry</i> , 2022, 33, 353-362.	3.6	6
41	Electronic Structures and OH-Induced Atmospheric Degradation of CF ₃ NSF ₂ : A Potential Green Dielectric Replacement for SF ₆ . <i>Journal of Physical Chemistry A</i> , 2017, 121, 2610-2619.	2.5	4
42	An Extended Multireference Study of the Singlet and Triplet States of the 9,10-didehydroanthracene Diradical. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3688-3696.	2.5	4
43	Solvent-dependent mechanistic aspects for the redox reaction of paraquat in basic solution. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26757.	2.0	4
44	Theoretical Investigations on the Hydroxyl-Initialized Oxidation of Hexafluoro-2-butyne in the Presence of Oxygen. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1994-2006.	2.5	4
45	Synthesis and dielectric properties of the eco-friendly insulating gas thiazyl trifluoride. <i>RSC Advances</i> , 2020, 10, 2740-2746.	3.6	3
46	ONIOM study of the nonbonding interaction of the 2PU inhibitor with the CDK2 and CDK4 cyclin-dependent kinases. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 1148-1157.	2.0	2
47	Theoretical study of corrosion inhibition on copper in transformer oil. , 2016, , .		2
48	Mechanistic insight into the Rh(III)-catalyzed cascade annulation of β -ethynylanilines with diazo compounds towards Benzo[a]carbazoles. <i>Journal of Organometallic Chemistry</i> , 2018, 876, 17-25.	1.8	2
49	Influence of glucose as a contaminant on discharge characteristics of HVAC insulator. <i>IEEE Transactions on Dielectrics and Electrical Insulation</i> , 2016, 23, 394-402.	2.9	1
50	Computational study on the hydrolysis of halomethanes. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	1.4	1
51	Structure-activity Relationship and Molecular Design for Discovery of Environmentally Sustainable Dielectric Gases. , 2020, , .		1
52	A Simple Group-Additivity Method to Predict the Dielectric Strength of Insulating Gases for Molecular Design. , 2021, , .		1
53	Stereo-dependent dimerization, boiling points, diffusion coefficients, and dielectric constants of E/Z- α -HFO-1234ze. <i>International Journal of Quantum Chemistry</i> , 0, , e26848.	2.0	1
54	H proton intramolecular transformation in OH-OO-isoprene radicals. <i>Computational and Theoretical Chemistry</i> , 2018, 1130, 63-67.	2.5	0

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55	Theoretical Investigations on the Decomposition Characteristic Gases of Fluoronitriles/CO ₂ Mixture After Arc Interruption. , 2020, , .		0
56	Theoretical Study of the Role of a Catalytic Water Molecule in the Hydrolysis of Thionyl Tetrafluoride (SOF ₄). Journal of Physical Chemistry A, 2020, 124, 5615-5620.	2.5	0
57	An Optimized Force Field for Vapor-Liquid Equilibria and Molecular Dynamics Simulations of Eco-Friendly Dielectric Fluid Perfluoronitriles. Journal of Physical Chemistry B, 2021, 125, 4465-4475.	2.6	0
58	Mechanistic Insight into the Decomposition of Eco-Friendly Dielectric Gas Heptafluoro-iso-butyronitrile in the Presence of Water Impurity. IEEE Transactions on Dielectrics and Electrical Insulation, 2021, 28, 1273-1281.	2.9	0
59	Prediction on the high-energy density covalent organic frameworks with diamond network. International Journal of Quantum Chemistry, 2021, 121, e26790.	2.0	0
60	Theoretical Investigations on the Mechanisms for Dielectric Failure of Heptafluoro-iso-butyronitrile in the Presence of Water Vapor. , 2021, , .		0