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	6-Iodopurine as a Versatile Building Block for RNA Purine Architecture Modifications. Bioconjugate Chemistry, 2022, 33, 353-362.	3.6	6
2	Theoretical Investigations on the Hydroxyl-Initialized Oxidation of Hexafluoro-2-butyne in the Presence of Oxygen. Journal of Physical Chemistry A, 2022, 126, 1994-2006.	2.5	4
3	An Optimized Force Field for Vaporâ€“Liquid Equilibria and Molecular Dynamics Simulations of Eco-Friendly Dielectric Fluid Perfluoronitriles. Journal of Physical Chemistry B, 2021, 125, 4465-4475.	2.6	0
4	Solventâ€dependent mechanistic aspects for the redox reaction of paraquat in basic solution. International Journal of Quantum Chemistry, 2021, 121, e26757.	2.0	4
5	Facile Synthesis of Polyphenothiazine as a Highâ€Performance pâ€Type Cathode for Rechargeable Lithium Batteries. ChemSusChem, 2021, 14, 3174-3181.	6.8	21
6	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
7	High-Performance Polymeric Lithium Salt Electrode Material from Phenolâ€“Formaldehyde Condensation. ACS Applied Materials & Interfaces, 2021, 13, 37289-37298.	8.0	15
8	Prediction on the highâ€energy density covalent organic frameworks with diamond network. International Journal of Quantum Chemistry, 2021, 121, e26790.	2.0	0
9	Covalent Organic Frameworks for Simultaneous CO2 Capture and Selective Catalytic Transformation. Catalysts, 2021, 11, 1133.	3.5	16
10	Fractal Analysis on Pore Structure and Hydration of Magnesium Oxysulfate Cements by First Principle, Thermodynamic and Microstructure-Based Methods. Fractal and Fractional, 2021, 5, 164.	3.3	111
11	A Simple Group-Additivity Method to Predict the Dielectric Strength of Insulating Gases for Molecular Design. , 2021, , .		1
12	Theoretical Investigations on the Mechanisms for Dielectric Failure of Heptafluoro-iso-butyronitrile in the Presence of Water Vapor. , 2021, , .		0
13	Phosphoric acid functionalized magnetic sorbents for selective enrichment of TiO2 nanoparticles in surface water followed by inductively coupled plasma mass spectrometry detection. Science of the Total Environment, 2020, 703, 135464.	8.0	9
14	Dielectric Properties of CF₃SO₂F/N₂ and CF₃SO₂F/CO₂ Mixtures as a Substitute to SF₆. Industrial & Engineering Chemistry Research, 2020, 59, 15796-15804.	3.7	15
15	Theoretical Investigations on the Decomposition Characteristic Gases of Fluoronitriles/CO2 Mixture After Arc Interruption. , 2020, , .		0
16	Theoretical Investigations on the Oxidation of Heptafluoro-iso-butyronitrile by Atomic Oxygen in Dielectric Breakdown. Journal of Physical Chemistry A, 2020, 124, 8398-8413.	2.5	6
17	Structure-activity Relationship and Molecular Design for Discovery of Environmentally Sustainable Dielectric Gases. , 2020, , .		1
18	Theoretical Study of the Role of a Catalytic Water Molecule in the Hydrolysis of Thionyl Tetrafluoride (SOF4). Journal of Physical Chemistry A, 2020, 124, 5615-5620.	2.5	0

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19	Development and application of a ReaxFF reactive force field for molecular dynamics of perfluorinatedketones thermal decomposition. Chemical Physics, 2020, 538, 110888.	1.9	14
20	ReaxFF reactive force field development and application for molecular dynamics simulations of heptafluoroisobutyronitrile thermal decomposition. Chemical Physics Letters, 2020, 751, 137554.	2.6	6
21	Synthesis and dielectric properties of the eco-friendly insulating gas thiazyl trifluoride. RSC Advances, 2020, 10, 2740-2746.	3.6	3
22	Surface Sensitive Photoluminescence of Carbon Nanodots: Coupling between the Carbonyl Group and Ï€-Electron System. Journal of Physical Chemistry Letters, 2019, 10, 3621-3629.	4.6	61
23	Synthesis and Dielectric Properties of Trifluoromethanesulfonyl Fluoride: An Alternative Gas to SF₆. Industrial & Engineering Chemistry Research, 2019, 58, 21913-21920.	3.7	21
24	Mechanisms of Modulation of Calcium Phosphate Pathological Mineralization by Mobile and Immobile Small-Molecule Inhibitors. Journal of Physical Chemistry B, 2018, 122, 1580-1587.	2.6	20
25	An Extended Multireference Study of the Singlet and Triplet States of the 9,10-didehydroanthracene Diradical. Journal of Physical Chemistry A, 2018, 122, 3688-3696.	2.5	4
26	H proton intramolecular transformation in OH-OO -isoprene radicals. Computational and Theoretical Chemistry, 2018, 1130, 63-67.	2.5	0
27	A Priori Theoretical Model for Discovery of Environmentally Sustainable Perfluorinated Compounds. Journal of Physical Chemistry A, 2018, 122, 3462-3469.	2.5	18
28	Computational study on the hydrolysis of halomethanes. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	1
29	An AIEgen-based 3D covalent organic framework for white light-emitting diodes. Nature Communications, 2018, 9, 5234.	12.8	293
30	Atmospheric Chemistry of Perfluoro-3-methyl-2-butanone [CF₃C(O)CF(CF₃)₂]: Photodissociation and Reaction with OH Radicals. Journal of Physical Chemistry A, 2018, 122, 8840-8848.	2.5	8
31	Mechanistic and Kinetic Investigations on the Thermal Unimolecular Reaction of Heptafluoroisobutyronitrile. Journal of Physical Chemistry A, 2018, 122, 7704-7715.	2.5	31
32	Mechanistic insight into the Rh(III)-catalyzed cascade annulation of Î¿-ethynylanilines with diazo compounds towards Benzo[a]carbazoles. Journal of Organometallic Chemistry, 2018, 876, 17-25.	1.8	2
33	Prediction on dielectric strength and boiling point of gaseous molecules for replacement of SF₆. Journal of Computational Chemistry, 2017, 38, 721-729.	3.3	47
34	3D Porphyrin-Based Covalent Organic Frameworks. Journal of the American Chemical Society, 2017, 139, 8705-8709.	13.7	369
35	Role of Alcoholic Hydroxyls of Dicarboxylic Acids in Regulating Nanoscale Dissolution Kinetics of Dicalcium Phosphate Dihydrate. ACS Sustainable Chemistry and Engineering, 2017, 5, 3920-3928.	6.7	16
36	Electronic Structures and OH-Induced Atmospheric Degradation of CF₃NSF₂: A Potential Green Dielectric Replacement for SF₆. Journal of Physical Chemistry A, 2017, 121, 2610-2619.	2.5	4

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37	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. Journal of Physical Chemistry A, 2017, 121, 9020-9032.	2.5	7
38	Preparation of Monodisperse Hydrophilic Quantum Dots with Amphiphilic Polymers. ACS Applied Materials & Interfaces, 2017, 9, 39901-39906.	8.0	17
39	A 2D porous porphyrin-based covalent organic framework for sulfur storage in lithiumâ€“sulfur batteries. Journal of Materials Chemistry A, 2016, 4, 7416-7421.	10.3	267
40	Influence of glucose as a contaminant on discharge characteristics of HVAC insulator. IEEE Transactions on Dielectrics and Electrical Insulation, 2016, 23, 394-402.	2.9	1
41	Theoretical study of corrosion inhibition on copper in transformer oil. , 2016, , .		2
42	Detection of intense partial discharge of epoxy insulation in sf6 insulated equipment using carbonyl sulfide. IEEE Transactions on Dielectrics and Electrical Insulation, 2016, 23, 2942-2948.	2.9	19
43	A Pyrene-Based, Fluorescent Three-Dimensional Covalent Organic Framework. Journal of the American Chemical Society, 2016, 138, 3302-3305.	13.7	628
44	Experimental and Theoretical Study on the OH-Reaction Kinetics and Photochemistry of Acetyl Fluoride (CH3C(O)F), an Atmospheric Degradation Intermediate of HFC-161 (C2H5F). Journal of Physical Chemistry A, 2015, 119, 7753-7765.	2.5	10
45	Theoretical study of the mechanisms and kinetics of the reactions of hydroperoxy (HO₂) radicals with hydroxymethylperoxy (HOCH₂O₂) and methoxymethylperoxy (CH₃OCH₂O₂) radicals. Physical Chemistry Chemical Physics, 2014, 16, 22805-22814.	2.8	12
46	Theoretical Study of the Adsorption/Dissociation Reactions of Formic Acid on the Î±-Al₂O₃(0001) Surface. Journal of Physical Chemistry C, 2014, 118, 20889-20898.	3.1	23
47	A Tetrathiafulvaleneâ€Based Electroactive Covalent Organic Framework. Chemistry - A European Journal, 2014, 20, 14614-14618.	3.3	143
48	Theoretical study of the hydrolysis of sulfur tetrafluoride. Journal of Fluorine Chemistry, 2013, 153, 114-120.	1.7	6
49	Insulation condition monitoring of epoxy spacers in GIS using a decomposed gas CS2. IEEE Transactions on Dielectrics and Electrical Insulation, 2013, 20, 2152-2157.	2.9	24
50	An improved B3LYP method in the calculation of organic thermochemistry and reactivity. Computational and Theoretical Chemistry, 2013, 1015, 64-71.	2.5	56
51	Extensive theoretical studies of a new energetic material: Tetrazinoâ€tetrazineâ€tetraoxide (TTTO). Journal of Computational Chemistry, 2009, 30, 1816-1820.	3.3	55
52	ONIOM study of the nonbonding interaction of the 2PU inhibitor with the CDK2 and CDK4 cyclinâ€dependant kinases. International Journal of Quantum Chemistry, 2009, 109, 1148-1157.	2.0	2
53	Ab initio study of the reaction of propionyl (C2H5CO) radical with oxygen (O2). Journal of Chemical Physics, 2007, 127, 054306.	3.0	61
54	Theoretical investigations on the SO2+HO2 reaction and the SO2â€“HO2 radical complex. Chemical Physics Letters, 2005, 410, 235-241.	2.6	48

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55	Mechanistic and kinetic study of the CH3CO+O2 reaction. Journal of Chemical Physics, 2005, 122, 224304.	3.0	34
56	A Systematic Computational Study of the Reactions of HO2 with RO2:â€‰ The HO2 + C2H5O2 Reaction. Journal of Physical Chemistry A, 2005, 109, 11206-11212.	2.5	31
57	A Systematic Computational Study on the Reactions of HO2 with RO2:â€‰ The HO2 + CH3O2(CD3O2) and HO2 + CH2FO2 Reactions. Journal of Physical Chemistry A, 2005, 109, 451-460.	2.5	56
58	A Systematic Computational Study of the Reactions of HO2 with RO2:â€‰ The HO2 + CH2ClO2, CHCl2O2, and CCl3O2 Reactions. Journal of Physical Chemistry A, 2005, 109, 9299-9309.	2.5	38
59	Computational Study of the Ionâ^'Molecule Reactions Involving Fluxional Cations:Â CH4++ H2â†' CH5++ H and Isotope Effect. Journal of Physical Chemistry A, 2005, 109, 8537-8547.	2.5	7
60	Stereoâ€dependent dimerization, boiling points, diffusion coefficients, and dielectric constants of E/Zâ€HFOâ€1234ze. International Journal of Quantum Chemistry, 0, , e26848.	2.0	1