

Junwei Lucas Bao

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

53
papers

2,107
citations

25
h-index

45
g-index

56
ext. papers

2,579
ext. citations

11.4
avg, IF

5.74
L-index

#	Paper	IF	Citations
53	Aqueous Mg-Ion Battery Based on Polyimide Anode and Prussian Blue Cathode. <i>ACS Energy Letters</i> , 2017 , 2, 1115-1121	20.1	207
52	Atmospheric Chemistry of Criegee Intermediates: Unimolecular Reactions and Reactions with Water. <i>Journal of the American Chemical Society</i> , 2016 , 138, 14409-14422	16.4	203
51	Variational transition state theory: theoretical framework and recent developments. <i>Chemical Society Reviews</i> , 2017 , 46, 7548-7596	58.5	186
50	Multiconfiguration Pair-Density Functional Theory: A New Way To Treat Strongly Correlated Systems. <i>Accounts of Chemical Research</i> , 2017 , 50, 66-73	24.3	175
49	Graphene-Supported Nitrogen and Boron Rich Carbon Layer for Improved Performance of Lithium Sulfur Batteries Due to Enhanced Chemisorption of Lithium Polysulfides. <i>Advanced Energy Materials</i> , 2016 , 6, 1501733	21.8	140
48	All-Organic Rechargeable Battery with Reversibility Supported by "Water-in-Salt" Electrolyte. <i>Chemistry - A European Journal</i> , 2017 , 23, 2560-2565	4.8	95
47	Self-Interaction Error in Density Functional Theory: An Appraisal. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 2353-2358	6.4	86
46	Multi-path variational transition state theory for chiral molecules: the site-dependent kinetics for abstraction of hydrogen from 2-butanol by hydroperoxyl radical, analysis of hydrogen bonding in the transition state, and dramatic temperature dependence of the activation energy. <i>Chemical Science</i> , 2015 , 6, 5866-5881	9.4	55
45	Unimolecular reaction of acetone oxide and its reaction with water in the atmosphere. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, 6135-6140	11.5	55
44	Rapid unimolecular reaction of stabilized Criegee intermediates and implications for atmospheric chemistry. <i>Nature Communications</i> , 2019 , 10, 2003	17.4	50
43	Kinetics of Hydrogen Radical Reactions with Toluene Including Chemical Activation Theory Employing System-Specific Quantum RRK Theory Calibrated by Variational Transition State Theory. <i>Journal of the American Chemical Society</i> , 2016 , 138, 2690-704	16.4	50
42	Reaction of SO with OH in the atmosphere. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 8091-8100	3.6	49
41	A versatile single-ion electrolyte with a Grotthuss-like Li conduction mechanism for dendrite-free Li metal batteries. <i>Energy and Environmental Science</i> , 2019 , 12, 2741-2750	35.4	49
40	Hydrogen Abstraction Reactions from Phenolic Compounds by Peroxyl Radicals: Multireference Character and Density Functional Theory Rate Constants. <i>Journal of Physical Chemistry A</i> , 2016 , 120, 4634-42	2.8	47
39	Predicting Bond Dissociation Energies of Transition-Metal Compounds by Multiconfiguration Pair-Density Functional Theory and Second-Order Perturbation Theory Based on Correlated Participating Orbitals and Separated Pairs. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 616-626	6.4	41
38	Correlated-Participating-Orbitals Pair-Density Functional Method and Application to Multiplet Energy Splittings of Main-Group Divalent Radicals. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 4274-83	6.4	41
37	Path-dependent variational effects and multidimensional tunneling in multi-path variational transition state theory: rate constants calculated for the reactions of HO ₂ with tert-butanol by including all 46 paths for abstraction at C and all six paths for abstraction at O. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 1032-41	3.6	39

36	On the Upper Limits of Oxidation States in Chemistry. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 3242-3245	16.4	37
35	Kinetics of the Strongly Correlated CHO + O Reaction: The Importance of Quadruple Excitations in Atmospheric and Combustion Chemistry. <i>Journal of the American Chemical Society</i> , 2019 , 141, 611-617	16.4	37
34	Predicting pressure-dependent unimolecular rate constants using variational transition state theory with multidimensional tunneling combined with system-specific quantum RRK theory: a definitive test for fluoroform dissociation. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 16659-70	3.6	30
33	Plasmon-driven carbon-fluorine (C(sp ³)) bond activation with mechanistic insights into hot-carrier-mediated pathways. <i>Nature Catalysis</i> , 2020 , 3, 564-573	36.5	29
32	Revisiting the designing criteria of advanced solid electrolyte interphase on lithium metal anode under practical condition. <i>Nano Energy</i> , 2021 , 83, 105847	17.1	29
31	Dual Lithiophilic Structure for Uniform Li Deposition. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 10616-10623	9.5	29
30	Surface-Plasmon-Induced Ammonia Decomposition on Copper: Excited-State Reaction Pathways Revealed by Embedded Correlated Wavefunction Theory. <i>ACS Nano</i> , 2019 , 13, 9944-9957	16.7	26
29	Density Functional Theory of the Water Splitting Reaction on Fe(0): Comparison of Local and Nonlocal Correlation Functionals. <i>ACS Catalysis</i> , 2015 , 5, 2070-2080	13.1	25
28	Degradation of Carbonyl Hydroperoxides in the Atmosphere and in Combustion. <i>Journal of the American Chemical Society</i> , 2017 , 139, 15821-15835	16.4	24
27	Anharmonicity of Coupled Torsions: The Extended Two-Dimensional Torsion Method and Its Use To Assess More Approximate Methods. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 3478-3492	6.4	22
26	Silane-initiated nucleation in chemically active plasmas: validation of density functionals, mechanisms, and pressure-dependent variational transition state calculations. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 10097-108	3.6	21
25	Multiconfiguration Pair-Density Functional Theory Is Free From Delocalization Error. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 5616-5620	6.4	21
24	Hydrogen shift isomerizations in the kinetics of the second oxidation mechanism of alkane combustion. Reactions of the hydroperoxypentylperoxy OOQOOH radical. <i>Combustion and Flame</i> , 2018 , 197, 88-101	5.3	20
23	Dual-Level Method for Estimating Multistructural Partition Functions with Torsional Anharmonicity. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 2511-2522	6.4	19
22	Nanodusty plasma chemistry: a mechanistic and variational transition state theory study of the initial steps of silyl anion-silane and silylene anion-silane polymerization reactions. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 15928-35	3.6	18
21	Barrierless association of CF ₂ and dissociation of C ₂ F ₄ by variational transition-state theory and system-specific quantum Rice-Ramsperger-Kassel theory. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016 , 113, 13606-13611	11.5	18
20	Predicting bond dissociation energy and bond length for bimetallic diatomic molecules: a challenge for electronic structure theory. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 5839-5854	3.6	16
19	Rationalizing the Hot-Carrier-Mediated Reaction Mechanisms and Kinetics for Ammonia Decomposition on Ruthenium-Doped Copper Nanoparticles. <i>Journal of the American Chemical Society</i> , 2019 , 141, 13320-13323	16.4	15

18	First-Principles Insights into Plasmon-Induced Catalysis. <i>Annual Review of Physical Chemistry</i> , 2021 , 72, 99-119	15.7	14
17	Theoretical Study of the Reaction Mechanism and Kinetics of HO ₂ with XCHO (X = F, Cl). <i>International Journal of Chemical Kinetics</i> , 2017 , 49, 130-139	1.4	12
16	Hot carrier multiplication in plasmonic photocatalysis. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021 , 118,	11.5	12
15	Enabling Lithium Metal Anode in Nonflammable Phosphate Electrolyte with Electrochemically Induced Chemical Reactions. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 19183-19190	16.4	11
14	Relative Rates of Hydrogen Shift Isomerizations Depend Strongly on Multiple-Structure Anharmonicity. <i>Journal of the American Chemical Society</i> , 2018 , 140, 17556-17570	16.4	11
13	Der Oxidationszahl-Obergrenzen in der Chemie. <i>Angewandte Chemie</i> , 2018 , 130, 3297-3300	3.6	10
12	How well can density functional theory and pair-density functional theory predict the correct atomic charges for dissociation and accurate dissociation energetics of ionic bonds?. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 23072-23078	3.6	10
11	Atmospheric Kinetics: Bimolecular Reactions of Carbonyl Oxide by a Triple-Level Strategy. <i>Journal of the American Chemical Society</i> , 2021 , 143, 8402-8413	16.4	6
10	Extended Hamiltonian molecular dynamics: semiclassical trajectories with improved maintenance of zero point energy. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 30209-30218	3.6	4
9	Effect of energy dependence of the density of states on pressure-dependent rate constants. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 30475-30479	3.6	4
8	Predicting Bond Dissociation Energies and Bond Lengths of Coordinatively Unsaturated Vanadium-Ligand Bonds. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 9757-9770	2.8	3
7	Large Pressure Effects Caused by Internal Rotation in the -Acrolein Stabilized Criegee Intermediate at Tropospheric Temperature and Pressure.. <i>Journal of the American Chemical Society</i> , 2022 ,	16.4	2
6	mad-GP: automatic differentiation of Gaussian processes for molecules and materials. <i>Journal of Mathematical Chemistry</i> , 1	2.1	2
5	Enabling Lithium Metal Anode in Nonflammable Phosphate Electrolyte with Electrochemically Induced Chemical Reactions. <i>Angewandte Chemie</i> , 2021 , 133, 19332-19339	3.6	1
4	Reaction of SO with HONO and Implications for Sulfur Partitioning in the Atmosphere.. <i>Journal of the American Chemical Society</i> , 2022 ,	16.4	1
3	CO ₂ Adsorptions on d-Block-Metal-Doped Nickel Nanoparticles: Unexpected Adsorption Configurations Predicted by Machine Intelligence. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 19839-19846	3.8	0
2	Geometry meta-optimization.. <i>Journal of Chemical Physics</i> , 2022 , 156, 134109	3.9	0
1	Innentitelbild: Enabling Lithium Metal Anode in Nonflammable Phosphate Electrolyte with Electrochemically Induced Chemical Reactions (Angew. Chem. 35/2021). <i>Angewandte Chemie</i> , 2021 , 133, 19042-19042	3.6	

