Junwei Lucas Bao

List of Publications by Year in Descending Order

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	Large Pressure Effects Caused by Internal Rotation in the -Acrolein Stabilized Criegee Intermediate at Tropospheric Temperature and Pressure.. *Journal of the American Chemical Society*, **2022**,	16.4	2
52	Geometry meta-optimization.. *Journal of Chemical Physics*, **2022**, 156, 134109	3.9	0
51	Reaction of SO with HONO and Implications for Sulfur Partitioning in the Atmosphere.. *Journal of the American Chemical Society*, **2022**,	16.4	1
50	Atmospheric Kinetics: Bimolecular Reactions of Carbonyl Oxide by a Triple-Level Strategy. *Journal of the American Chemical Society*, **2021**, 143, 8402-8413	16.4	6
49	Revisiting the designing criteria of advanced solid electrolyte interphase on lithium metal anode under practical condition. *Nano Energy*, **2021**, 83, 105847	17.1	29
48	Hot carrier multiplication in plasmonic photocatalysis. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	12
47	Innentitelbild: Enabling Lithium Metal Anode in Nonflammable Phosphate Electrolyte with Electrochemically Induced Chemical Reactions (Angew. Chem. 35/2021). *Angewandte Chemie*, **2021**, 133, 19042-19042	3.6	
46	Enabling Lithium Metal Anode in Nonflammable Phosphate Electrolyte with Electrochemically Induced Chemical Reactions. *Angewandte Chemie - International Edition*, **2021**, 60, 19183-19190	16.4	11
45	Enabling Lithium Metal Anode in Nonflammable Phosphate Electrolyte with Electrochemically Induced Chemical Reactions. *Angewandte Chemie*, **2021**, 133, 19332-19339	3.6	1
44	First-Principles Insights into Plasmon-Induced Catalysis. *Annual Review of Physical Chemistry*, **2021**, 72, 99-119	15.7	14
43	CO2 Adsorptions on d-Block-Metal-Doped Nickel Nanoparticles: Unexpected Adsorption Configurations Predicted by Machine Intelligence. *Journal of Physical Chemistry C*, **2021**, 125, 19839-19846	3.8	0
42	Plasmon-driven carbon□luorine (C(sp3)□) bond activation with mechanistic insights into hot-carrier-mediated pathways. *Nature Catalysis*, **2020**, 3, 564-573	36.5	29
41	Predicting Bond Dissociation Energies and Bond Lengths of Coordinatively Unsaturated Vanadium-Ligand Bonds. *Journal of Physical Chemistry A*, **2020**, 124, 9757-9770	2.8	3
40	Rapid unimolecular reaction of stabilized Criegee intermediates and implications for atmospheric chemistry. *Nature Communications*, **2019**, 10, 2003	17.4	50
39	Rationalizing the Hot-Carrier-Mediated Reaction Mechanisms and Kinetics for Ammonia Decomposition on Ruthenium-Doped Copper Nanoparticles. *Journal of the American Chemical Society*, **2019**, 141, 13320-13323	16.4	15
38	Surface-Plasmon-Induced Ammonia Decomposition on Copper: Excited-State Reaction Pathways Revealed by Embedded Correlated Wavefunction Theory. *ACS Nano*, **2019**, 13, 9944-9957	16.7	26
37	A versatile single-ion electrolyte with a Grotthuss-like Li conduction mechanism for dendrite-free Li metal batteries. *Energy and Environmental Science*, **2019**, 12, 2741-2750	35.4	49

36	Dual Lithiophilic Structure for Uniform Li Deposition. *ACS Applied Materials & Interfaces*, **2019**, 11, 10616-10623	9.5	29
35	Kinetics of the Strongly Correlated CHO + O Reaction: The Importance of Quadruple Excitations in Atmospheric and Combustion Chemistry. *Journal of the American Chemical Society*, **2019**, 141, 611-617	16.4	37
34	Self-Interaction Error in Density Functional Theory: An Appraisal. *Journal of Physical Chemistry Letters*, **2018**, 9, 2353-2358	6.4	86
33	Über Oxidationszahl-Obergrenzen in der Chemie. *Angewandte Chemie*, **2018**, 130, 3297-3300	3.6	10
32	On the Upper Limits of Oxidation States in Chemistry. *Angewandte Chemie - International Edition*, **2018**, 57, 3242-3245	16.4	37
31	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?. *Physical Chemistry Chemical Physics*, **2018**, 20, 23072-23078	3.6	10
30	Hydrogen shift isomerizations in the kinetics of the second oxidation mechanism of alkane combustion. Reactions of the hydroperoxypentylperoxy OOQOOH radical. *Combustion and Flame*, **2018**, 197, 88-101	5.3	20
29	Extended Hamiltonian molecular dynamics: semiclassical trajectories with improved maintenance of zero point energy. *Physical Chemistry Chemical Physics*, **2018**, 20, 30209-30218	3.6	4
28	Effect of energy dependence of the density of states on pressure-dependent rate constants. *Physical Chemistry Chemical Physics*, **2018**, 20, 30475-30479	3.6	4
27	Relative Rates of Hydrogen Shift Isomerizations Depend Strongly on Multiple-Structure Anharmonicity. *Journal of the American Chemical Society*, **2018**, 140, 17556-17570	16.4	11
26	Unimolecular reaction of acetone oxide and its reaction with water in the atmosphere. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 6135-6140	11.5	55
25	All-Organic Rechargeable Battery with Reversibility Supported by "Water-in-Salt" Electrolyte. *Chemistry - A European Journal*, **2017**, 23, 2560-2565	4.8	95
24	Predicting bond dissociation energy and bond length for bimetallic diatomic molecules: a challenge for electronic structure theory. *Physical Chemistry Chemical Physics*, **2017**, 19, 5839-5854	3.6	16
23	Reaction of SO with OH in the atmosphere. *Physical Chemistry Chemical Physics*, **2017**, 19, 8091-8100	3.6	49
22	Aqueous Mg-Ion Battery Based on Polyimide Anode and Prussian Blue Cathode. *ACS Energy Letters*, **2017**, 2, 1115-1121	20.1	207
21	Dual-Level Method for Estimating Multistructural Partition Functions with Torsional Anharmonicity. *Journal of Chemical Theory and Computation*, **2017**, 13, 2511-2522	6.4	19
20	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. *Journal of Chemical Theory and Computation*, **2017**, 13, 616-626	6.4	41
19	Theoretical Study of the Reaction Mechanism and Kinetics of HO2 with XCHO (X = F, Cl). *International Journal of Chemical Kinetics*, **2017**, 49, 130-139	1.4	12

18	Multiconfiguration Pair-Density Functional Theory: A New Way To Treat Strongly Correlated Systems. *Accounts of Chemical Research*, **2017**, 50, 66-73	24.3	175
17	Degradation of Carbonyl Hydroperoxides in the Atmosphere and in Combustion. *Journal of the American Chemical Society*, **2017**, 139, 15821-15835	16.4	24
16	Variational transition state theory: theoretical framework and recent developments. *Chemical Society Reviews*, **2017**, 46, 7548-7596	58.5	186
15	Multiconfiguration Pair-Density Functional Theory Is Free From Delocalization Error. *Journal of Physical Chemistry Letters*, **2017**, 8, 5616-5620	6.4	21
14	Anharmonicity of Coupled Torsions: The Extended Two-Dimensional Torsion Method and Its Use To Assess More Approximate Methods. *Journal of Chemical Theory and Computation*, **2017**, 13, 3478-3492	6.4	22
13	Barrierless association of CF2 and dissociation of C2F4 by variational transition-state theory and system-specific quantum Rice-Ramsperger-Kassel theory. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 13606-13611	11.5	18
12	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. *Physical Chemistry Chemical Physics*, **2016**, 18, 16659-70	3.6	30
11	Kinetics of Hydrogen Radical Reactions with Toluene Including Chemical Activation Theory Employing System-Specific Quantum RRK Theory Calibrated by Variational Transition State Theory. *Journal of the American Chemical Society*, **2016**, 138, 2690-704	16.4	50
10	Silane-initiated nucleation in chemically active plasmas: validation of density functionals, mechanisms, and pressure-dependent variational transition state calculations. *Physical Chemistry Chemical Physics*, **2016**, 18, 10097-108	3.6	21
9	Path-dependent variational effects and multidimensional tunneling in multi-path variational transition state theory: rate constants calculated for the reactions of HO2 with tert-butanol by including all 46 paths for abstraction at C and all six paths for abstraction at O. *Physical Chemistry Chemical Physics*, **2016**, 18, 1032-41	3.6	39
8	Hydrogen Abstraction Reactions from Phenolic Compounds by Peroxyl Radicals: Multireference Character and Density Functional Theory Rate Constants. *Journal of Physical Chemistry A*, **2016**, 120, 4634-42	2.8	47
7	Graphene-Supported Nitrogen and Boron Rich Carbon Layer for Improved Performance of Lithium–Sulfur Batteries Due to Enhanced Chemisorption of Lithium Polysulfides. *Advanced Energy Materials*, **2016**, 6, 1501733	21.8	140
6	Atmospheric Chemistry of Criegee Intermediates: Unimolecular Reactions and Reactions with Water. *Journal of the American Chemical Society*, **2016**, 138, 14409-14422	16.4	203
5	Correlated-Participating-Orbitals Pair-Density Functional Method and Application to Multiplet Energy Splittings of Main-Group Divalent Radicals. *Journal of Chemical Theory and Computation*, **2016**, 12, 4274-83	6.4	41
4	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. *Chemical Science*, **2015**, 6, 5866-5881	9.4	55
3	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. *Physical Chemistry Chemical Physics*, **2015**, 17, 15928-35	3.6	18
2	Density Functional Theory of the Water Splitting Reaction on Fe(0): Comparison of Local and Nonlocal Correlation Functionals. *ACS Catalysis*, **2015**, 5, 2070-2080	13.1	25
1	mad-GP: automatic differentiation of Gaussian processes for molecules and materials. *Journal of Mathematical Chemistry*,1	2.1	2