Junwei Lucas Bao

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4773812/publications.pdf

Version: 2024-02-01

54 papers	3,065 citations	159358 30 h-index	174990 52 g-index
56 all docs	56 docs citations	56 times ranked	3601 citing authors

#	Article	IF	Citations
1	Aqueous Mg-Ion Battery Based on Polyimide Anode and Prussian Blue Cathode. ACS Energy Letters, 2017, 2, 1115-1121.	8.8	283
2	Variational transition state theory: theoretical framework and recent developments. Chemical Society Reviews, 2017, 46, 7548-7596.	18.7	281
3	Atmospheric Chemistry of Criegee Intermediates: Unimolecular Reactions and Reactions with Water. Journal of the American Chemical Society, 2016, 138, 14409-14422.	6.6	265
4	Multiconfiguration Pair-Density Functional Theory: A New Way To Treat Strongly Correlated Systems. Accounts of Chemical Research, 2017, 50, 66-73.	7.6	232
5	Grapheneâ€Supported Nitrogen and Boron Rich Carbon Layer for Improved Performance of Lithiumâ€“Sulfur Batteries Due to Enhanced Chemisorption of Lithium Polysulfides. Advanced Energy Materials, 2016, 6, 1501733.	10.2	162
6	Self-Interaction Error in Density Functional Theory: An Appraisal. Journal of Physical Chemistry Letters, 2018, 9, 2353-2358.	2.1	131
7	Allâ€Organic Rechargeable Battery with Reversibility Supported by â€œWaterâ€in‐â€Saltâ€•Electrolyte. Chemistry - A European Journal, 2017, 23, 2560-2565.	1.7	111
8	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.	15.6	89
9	Plasmon-driven carbonâ€“fluorine (C(sp3)â€“F) bond activation with mechanistic insights into hot-carrier-mediated pathways. Nature Catalysis, 2020, 3, 564-573.	16.1	81
10	Revisiting the designing criteria of advanced solid electrolyte interphase on lithium metal anode under practical condition. Nano Energy, 2021, 83, 105847.	8.2	79
11	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.	3.3	76
12	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, 2690-2704.	6.6	72
13	Rapid unimolecular reaction of stabilized Criegee intermediates and implications for atmospheric chemistry. Nature Communications, 2019, 10, 2003.	5.8	72
14	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.	3.7	70
15	Reaction of SO₂with OH in the atmosphere. Physical Chemistry Chemical Physics, 2017, 19, 8091-8100.	1.3	63
16	Kinetics of the Strongly Correlated CH₃O + O₂ Reaction: The Importance of Quadruple Excitations in Atmospheric and Combustion Chemistry. Journal of the American Chemical Society, 2019, 141, 611-617.	6.6	59
17	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, 4274-4283.	2.3	55
18	Hydrogen Abstraction Reactions from Phenolic Compounds by Peroxyl Radicals: Multireference Character and Density Functional Theory Rate Constants. Journal of Physical Chemistry A, 2016, 120, 4634-4642.	1.1	55

#	Article	IF	Citations
19	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, 1032-1041.	1.3	48
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.	2.3	47
21	On the Upper Limits of Oxidation States in Chemistry. Angewandte Chemie - International Edition, 2018, 57, 3242-3245.	7.2	46
22	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, 16659-16670.	1.3	44
23	Dual Lithiophilic Structure for Uniform Li Deposition. ACS Applied Materials & Interfaces, 2019, 11, 10616-10623.	4.0	43
24	Hot carrier multiplication in plasmonic photocatalysis. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	43
25	First-Principles Insights into Plasmon-Induced Catalysis. Annual Review of Physical Chemistry, 2021, 72, 99-119.	4.8	41
26	Surface-Plasmon-Induced Ammonia Decomposition on Copper: Excited-State Reaction Pathways Revealed by Embedded Correlated Wavefunction Theory. ACS Nano, 2019, 13, 9944-9957.	7.3	38
27	Atmospheric Kinetics: Bimolecular Reactions of Carbonyl Oxide by a Triple-Level Strategy. Journal of the American Chemical Society, 2021, 143, 8402-8413.	6.6	36
28	Enabling Lithium Metal Anode in Nonflammable Phosphate Electrolyte with Electrochemically Induced Chemical Reactions. Angewandte Chemie - International Edition, 2021, 60, 19183-19190.	7.2	36
29	Degradation of Carbonyl Hydroperoxides in the Atmosphere and in Combustion. Journal of the American Chemical Society, 2017, 139, 15821-15835.	6.6	34
30	Multiconfiguration Pair-Density Functional Theory Is Free From Delocalization Error. Journal of Physical Chemistry Letters, 2017, 8, 5616-5620.	2.1	31
31	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.	2.3	30
32	Dual-Level Method for Estimating Multistructural Partition Functions with Torsional Anharmonicity. Journal of Chemical Theory and Computation, 2017, 13, 2511-2522.	2.3	29
33	Density Functional Theory of the Water Splitting Reaction on Fe(0): Comparison of Local and Nonlocal Correlation Functionals. ACS Catalysis, 2015, 5, 2070-2080.	5.5	28
34	Barrierless association of CF ₂ and dissociation of C ₂ F ₄ by variational transition-state theory and system-specific quantum Riceâ€“Ramspergerâ€“Kassel theory. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 13606-13611.	3.3	28
35	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, 10097-10108.	1.3	28
36	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.	6.6	25

#	Article	IF	Citations
37	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.	2.8	24
38	Nanodusty plasma chemistry: a mechanistic and variational transition state theory study of the initial steps of silyl anionâ€“silane and silylene anionâ€“silane polymerization reactions. Physical Chemistry Chemical Physics, 2015, 17, 15928-15935.	1.3	21
39	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.	1.3	21
40	Ãœber Oxidationszahlâ€Obergrenzen in der Chemie. Angewandte Chemie, 2018, 130, 3297-3300.	1.6	15
41	Relative Rates of Hydrogen Shift Isomerizations Depend Strongly on Multiple-Structure Anharmonicity. Journal of the American Chemical Society, 2018, 140, 17556-17570.	6.6	14
42	Theoretical Study of the Reaction Mechanism and Kinetics of HO₂ with XCHO (X = F, Cl). International Journal of Chemical Kinetics, 2017, 49, 130-139.	1.0	13
43	Large Pressure Effects Caused by Internal Rotation in the s-cis-syn-Acrolein Stabilized Criegee Intermediate at Tropospheric Temperature and Pressure. Journal of the American Chemical Society, 2022, 144, 4828-4838.	6.6	13
44	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.	1.3	11
45	Reaction of SO₃ with HONO₂ and Implications for Sulfur Partitioning in the Atmosphere. Journal of the American Chemical Society, 2022, 144, 9172-9177.	6.6	8
46	mad-GP: automatic differentiation of Gaussian processes for molecules and materials. Journal of Mathematical Chemistry, 0, , 1.	0.7	7
47	Extended Hamiltonian molecular dynamics: semiclassical trajectories with improved maintenance of zero point energy. Physical Chemistry Chemical Physics, 2018, 20, 30209-30218.	1.3	6
48	Effect of energy dependence of the density of states on pressure-dependent rate constants. Physical Chemistry Chemical Physics, 2018, 20, 30475-30479.	1.3	6
49	Predicting Bond Dissociation Energies and Bond Lengths of Coordinatively Unsaturated Vanadiumâ€“Ligand Bonds. Journal of Physical Chemistry A, 2020, 124, 9757-9770.	1.1	5
50	Geometry meta-optimization. Journal of Chemical Physics, 2022, 156, 134109.	1.2	4
51	Molecular-Level Insights into Selective Transport of Mg²⁺ in Metalâ€“Organic Frameworks. ACS Applied Materials & Interfaces, 2021, 13, 51974-51987.	4.0	3
52	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.	1.5	2
53	Enabling Lithium Metal Anode in Nonflammable Phosphate Electrolyte with Electrochemically Induced Chemical Reactions. Angewandte Chemie, 2021, 133, 19332-19339.	1.6	1
54	Innentitelbild: Enabling Lithium Metal Anode in Nonflammable Phosphate Electrolyte with Electrochemically Induced Chemical Reactions (Angew. Chem. 35/2021). Angewandte Chemie, 2021, 133, 19042-19042.	1.6	0