Paul M Zimmerman

List of Publications by Year
in descending order

122 papers	8,626 citations	66234 42 h-index	45213 90 g-index
124 all docs	124 docs citations	124 times ranked	8178 citing authors

#	Article	IF	Citations
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
2	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
3	Mechanism for Singlet Fission in Pentacene and Tetracene: From Single Exciton to Two Triplets. Journal of the American Chemical Society, 2011, 133, 19944-19952.	6.6	397
4	Singlet fission in pentacene through multi-exciton quantum states. Nature Chemistry, 2010, 2, 648-652.	6.6	356
5	Automated discovery of chemically reasonable elementary reaction steps. Journal of Computational Chemistry, 2013, 34, 1385-1392.	1.5	179
6	Iron(III)-catalysed carbonylâ€“olefin metathesis. Nature, 2016, 533, 374-379.	13.7	179
7	Reliable Transition State Searches Integrated with the Growing String Method. Journal of Chemical Theory and Computation, 2013, 9, 3043-3050.	2.3	177
8	Methods for exploring reaction space in molecular systems. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1354.	6.2	164
9	Singleâ€ended transition state finding with the growing string method. Journal of Computational Chemistry, 2015, 36, 601-611.	1.5	160
10	Efficient exploration of reaction paths via a freezing string method. Journal of Chemical Physics, 2011, 135, 224108.	1.2	154
11	A Correlated Electron View of Singlet Fission. Accounts of Chemical Research, 2013, 46, 1339-1347.	7.6	150
12	Growing string method with interpolation and optimization in internal coordinates: Method and examples. Journal of Chemical Physics, 2013, 138, 184102.	1.2	145
13	The Role of Free Nâ€Heterocyclic Carbene (NHC) in the Catalytic Dehydrogenation of Ammoniaâ€“Borane in the Nickel NHC System. Angewandte Chemie - International Edition, 2009, 48, 2201-2205.	7.2	115
14	Oligomerization and Autocatalysis of NH2BH2 with Ammoniaâˆ’Borane. Inorganic Chemistry, 2009, 48, 1069-1081.	1.9	108
15	Studies of the Mechanism and Origins of Enantioselectivity for the Chiral Phosphoric Acid-Catalyzed Stereoselective Spiroketalization Reactions. Journal of the American Chemical Society, 2016, 138, 444-456.	6.6	89
16	Incremental full configuration interaction. Journal of Chemical Physics, 2017, 146, 104102.	1.2	86
17	Navigating molecular space for reaction mechanisms: an efficient, automated procedure. Molecular Simulation, 2015, 41, 43-54.	0.9	82
18	Excited States of Methylene, Polyenes, and Ozone from Heat-Bath Configuration Interaction. Journal of Physical Chemistry A, 2018, 122, 2714-2722.	1.1	80

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19	Coupled double triplet state in singlet fission. Physical Chemistry Chemical Physics, 2018, 20, 30083-30094.	1.3	80
20	Experimental and Computational Assessment of Reactivity and Mechanism in C(sp³)â€“N Bond-Forming Reductive Elimination from Palladium(IV). Journal of the American Chemical Society, 2016, 138, 6049-6060.	6.6	79
21	Mechanistic Investigations of the Iron(III)-Catalyzed Carbonyl-Olefin Metathesis Reaction. Journal of the American Chemical Society, 2017, 139, 10832-10842.	6.6	77
22	Catalytic Dehydrogenation of Ammonia Borane at Ni Monocarbene and Dicarbene Catalysts. Inorganic Chemistry, 2009, 48, 5418-5433.	1.9	72
23	Highly Active Nickel Catalysts for Câ€“H Functionalization Identified through Analysis of Off-Cycle Intermediates. Journal of the American Chemical Society, 2015, 137, 7636-7639.	6.6	71
24	Excited states of methylene from quantum Monte Carlo. Journal of Chemical Physics, 2009, 131, 124103.	1.2	70
25	Simultaneous Two-Hydrogen Transfer as a Mechanism for Efficient CO₂ Reduction. Inorganic Chemistry, 2010, 49, 8724-8728.	1.9	70
26	Restricted active space spin-flip configuration interaction: Theory and examples for multiple spin flips with odd numbers of electrons. Journal of Chemical Physics, 2012, 137, 164110.	1.2	69
27	Selection and Validation of Charge and Lennard-Jones Parameters for QM/MM Simulations of Hydrocarbon Interactions with Zeolites. Journal of Chemical Theory and Computation, 2011, 7, 1695-1703.	2.3	67
28	Finding reaction mechanisms, intuitive or otherwise. Organic and Biomolecular Chemistry, 2017, 15, 501-504.	1.5	65
29	Restricted active space spin-flip (RAS-SF) with arbitrary number of spin-flips. Physical Chemistry Chemical Physics, 2013, 15, 358-366.	1.3	64
30	Regiodivergent Glycosylations of 6-Deoxy-erythronolide B and Oleandomycin-Derived Macrolactones Enabled by Chiral Acid Catalysis. Journal of the American Chemical Society, 2017, 139, 8570-8578.	6.6	63
31	Isospecific, Chain Shuttling Polymerization of Propylene Oxide Using a Bimetallic Chromium Catalyst: A New Route to Semicrystalline Polyols. Journal of the American Chemical Society, 2017, 139, 11048-11054.	6.6	63
32	Catalytic Carbonyl-Olefin Metathesis of Aliphatic Ketones: Iron(III) Homo-Dimers as Lewis Acidic Superelectrophiles. Journal of the American Chemical Society, 2019, 141, 1690-1700.	6.6	63
33	Enantioselective Synthesis of Piperidines through the Formation of Chiral Mixed Phosphoric Acid Acetals: Experimental and Theoretical Studies. Angewandte Chemie - International Edition, 2014, 53, 11194-11198.	7.2	59
34	Structure and Dynamics of the ¹(TT) State in a Quinoidal Bithiophene: Characterizing a Promising Intramolecular Singlet Fission Candidate. Journal of Physical Chemistry C, 2015, 119, 28258-28268.	1.5	56
35	The Mechanism of Acceptorless Amine Double Dehydrogenation by N,N,N-Amide Ruthenium(II) Hydrides: A Combined Experimental and Computational Study. ACS Catalysis, 2016, 6, 4799-4813.	5.5	56
36	Exact exchange-correlation potentials from ground-state electron densities. Nature Communications, 2019, 10, 4497.	5.8	54

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37	New Direct Approach for Determining the Reverse Intersystem Crossing Rate in Organic Thermally Activated Delayed Fluorescent (TADF) Emitters. Journal of the American Chemical Society, 2020, 142, 8074-8079.	6.6	52
38	Charge Transfer and Aggregation Effects on the Performance of Planar vs Twisted Nonfullerene Acceptor Isomers for Organic Solar Cells. Chemistry of Materials, 2018, 30, 4263-4276.	3.2	49
39	Entrances, Traps, and Rate-Controlling Factors for Nickel-Catalyzed Câ€“H Functionalization. ACS Catalysis, 2017, 7, 7352-7362.	5.5	48
40	Unraveling the Crucial Role of Metal-Free Catalysis in Borazine and Polyborazylene Formation in Transition-Metal-Catalyzed Ammoniaâ€“Borane Dehydrogenation. ACS Catalysis, 2015, 5, 3478-3493.	5.5	47
41	Interrupted carbonyl-olefin metathesis via oxygen atom transfer. Science, 2018, 361, 1363-1369.	6.0	47
42	Strong correlation in incremental full configuration interaction. Journal of Chemical Physics, 2017, 146, 224104.	1.2	46
43	Enacting Two-Electron Transfer from a Double-Triplet State of Intramolecular Singlet Fission. Journal of the American Chemical Society, 2018, 140, 7760-7763.	6.6	46
44	Fluoride Migration Catalysis Enables Simple, Stereoselective, and Iterative Glycosylation. Journal of the American Chemical Society, 2020, 142, 7235-7242.	6.6	43
45	Singletâ€“Triplet Gaps through Incremental Full Configuration Interaction. Journal of Physical Chemistry A, 2017, 121, 4712-4720.	1.1	42
46	Achieving Accurate Reduction Potential Predictions for Anthraquinones in Water and Aprotic Solvents: Effects of Inter- and Intramolecular H-Bonding and Ion Pairing. Journal of Physical Chemistry C, 2016, 120, 22235-22247.	1.5	41
47	Reliable and efficient reaction path and transition state finding for surface reactions with the growing string method. Journal of Computational Chemistry, 2017, 38, 645-658.	1.5	40
48	Recovering dynamic correlation in spin flip configuration interaction through a difference dedicated approach. Journal of Chemical Physics, 2017, 146, 014103.	1.2	38
49	Chemoenzymatic o-Quinone Methide Formation. Journal of the American Chemical Society, 2019, 141, 20269-20277.	6.6	38
50	Functionalized and Degradable Polyphthalaldehyde Derivatives. Journal of the American Chemical Society, 2019, 141, 14544-14548.	6.6	37
51	Learning To Predict Reaction Conditions: Relationships between Solvent, Molecular Structure, and Catalyst. Journal of Chemical Information and Modeling, 2019, 59, 3645-3654.	2.5	36
52	Mechanochemical Release of Nâ€Heterocyclic Carbenes from Flexâ€Activated Mechanophores. Angewandte Chemie - International Edition, 2021, 60, 13559-13563.	7.2	36
53	Fully Conjugated [4]Chrysaorene. Redox-Coupled Anion Binding in a Tetraradicaloid Macrocycle. Journal of the American Chemical Society, 2018, 140, 14474-14480.	6.6	35
54	Impact of Preferential Ï€-Binding in Catalyst-Transfer Polycondensation of Thiazole Derivatives. ACS Macro Letters, 2016, 5, 1411-1415.	2.3	33

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55	Simulated Mechanism for Palladium-Catalyzed, Directed Î³-Arylation of Piperidine. ACS Catalysis, 2017, 7, 5466-5477.	5.5	33
56	5,10-Dimesityldiindeno[1,2-a:2â€²,1â€²-i]phenanthrene: a stable biradicaloid derived from Chichibabin's hydrocarbon. Chemical Science, 2019, 10, 3413-3420.	3.7	33
57	Increasing the CO₂ Reduction Activity of Cobalt Phthalocyanine by Modulating the Ïƒ-Donor Strength of Axially Coordinating Ligands. ACS Catalysis, 2021, 11, 13203-13216.	5.5	33
58	Giving superabsorbent polymers a second life as pressure-sensitive adhesives. Nature Communications, 2021, 12, 4524.	5.8	32
59	Hexane Cracking on ZSM-5 and Faujasite Zeolites: a QM/MM/QCT Study. Journal of Physical Chemistry C, 2015, 119, 28836-28853.	1.5	31
60	Exploring the relationship between vibrational mode locality and coupling using constrained optimization. Journal of Chemical Physics, 2016, 144, 124111.	1.2	29
61	Optimizing Vibrational Coordinates To Modulate Intermode Coupling. Journal of Chemical Theory and Computation, 2016, 12, 1883-1891.	2.3	29
62	Evaluating the Effect of Heteroatoms on the Photophysical Properties of Donorâ€“Acceptor Conjugated Polymers Based on 2,6-Di(thiophen-2-yl)benzo[1,2-b:4,5-bâ€²]difuran: Two-Photon Cross-Section and Ultrafast Time-Resolved Spectroscopy. Journal of Physical Chemistry C, 2017, 121, 14382-14392.	1.5	27
63	On the nature of electron correlation in C60. Journal of Chemical Physics, 2011, 135, 194306.	1.2	26
64	Evaluation of full valence correlation energies and gradients. Journal of Chemical Physics, 2019, 150, 244117.	1.2	26
65	Predicting and Controlling Entangled Two-Photon Absorption in Diatomic Molecules. Journal of Physical Chemistry A, 2018, 122, 8198-8212.	1.1	25
66	Revealing the Strong Relationships between Ligand Conformers and Activation Barriers: A Case Study of Bisphosphine Reductive Elimination. ACS Catalysis, 2020, 10, 7136-7145.	5.5	25
67	Metalâ€Free Organic Triplet Emitters with Onâ€“Off Switchable Excited State Intramolecular Proton Transfer. Advanced Functional Materials, 2022, 32, .	7.8	25
68	Discovery of conical intersection mediated photochemistry with growing string methods. Physical Chemistry Chemical Physics, 2018, 20, 27394-27405.	1.3	24
69	Virtual Screening of Hole Transport, Electron Transport, and Host Layers for Effective OLED Design. Journal of Chemical Information and Modeling, 2018, 58, 2440-2449.	2.5	22
70	Activating intramolecular singlet exciton fission by altering Ï€-bridge flexibility in perylene diimide trimers for organic solar cells. Chemical Science, 2020, 11, 8757-8770.	3.7	22
71	Computational Mechanism for Initiation and Growth of Poly(3-hexylthiophene) Using Palladium N-Heterocyclic Carbene Precatalysts. Macromolecules, 2016, 49, 7632-7641.	2.2	21
72	Predicting reaction conditions from limited data through active transfer learning. Chemical Science, 2022, 13, 6655-6668.	3.7	21

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73	Mechanistic Insight into Thiophene Catalyst-Transfer Polymerization Mediated by Nickel Diimine Catalysts. Macromolecules, 2017, 50, 9121-9127.	2.2	20
74	Examining the Ways To Bend and Break Reaction Pathways Using Mechanochemistry. Journal of Physical Chemistry C, 2018, 122, 6996-7004.	1.5	20
75	Spin-Switching Transmetalation at Ni Diimine Catalysts. ACS Catalysis, 2018, 8, 3655-3666.	5.5	20
76	Heteroatom and Side Chain Effects on the Optical and Photophysical Properties: Ultrafast and Nonlinear Spectroscopy of New Naphtho[1,2-b:5,6-bâ€²]difuran Donor Polymers. Journal of Physical Chemistry C, 2018, 122, 17049-17066.	1.5	20
77	What Does the Machine Learn? Knowledge Representations of Chemical Reactivity. Journal of Chemical Information and Modeling, 2020, 60, 1290-1301.	2.5	19
78	Calculation of spinâ€“orbit couplings using RASCI spinless one-particle density matrices: Theory and applications. Journal of Chemical Physics, 2020, 153, 214107.	1.2	18
79	Heavy atom oriented orbital angular momentum manipulation in metal-free organic phosphors. Chemical Science, 2022, 13, 789-797.	3.7	18
80	Using ultra-fast spectroscopy to probe the excited state dynamics of a reported highly efficient thermally activated delayed fluorescence chromophore. Journal of Materials Chemistry C, 2019, 7, 4210-4221.	2.7	16
81	Mechanism for Forming B,C,N,O Rings from NH₃BH₃ and CO₂ via Reaction Discovery Computations. Journal of Physical Chemistry A, 2016, 120, 1135-1144.	1.1	15
82	Ligand-Induced Reductive Elimination of Ethane from Azopyridine Palladium Dimethyl Complexes. Journal of the American Chemical Society, 2018, 140, 11408-11415.	6.6	15
83	An Openâ€Shell Coronoid with Hybrid Chichibabinâ€“Schlenk Conjugation. Angewandte Chemie - International Edition, 2021, 60, 22496-22504.	7.2	15
84	Density Functional Physicality in Electronic Coupling Estimation: Benchmarks and Error Analysis. Journal of Physical Chemistry Letters, 2017, 8, 3242-3248.	2.1	14
85	An Ionâ€Pairing Approach to Stereoselective Metalâ€Free Ringâ€Opening Metathesis Polymerization. Angewandte Chemie - International Edition, 2021, 60, 13952-13958.	7.2	14
86	An Unusual Iron-Dependent Oxidative Deformylation Reaction Providing Insight into Hydrocarbon Biosynthesis in Nature. ACS Catalysis, 2016, 6, 3293-3300.	5.5	13
87	Mechanistic Study of Isotactic Poly(propylene oxide) Synthesis using a Tethered Bimetallic Chromium Salen Catalyst. ACS Catalysis, 2020, 10, 8960-8967.	5.5	13
88	A Comparison of Exact and Model Exchangeâ€“Correlation Potentials for Molecules. Journal of Physical Chemistry Letters, 2021, 12, 12012-12019.	2.1	13
89	Hydroxyl Radical-Coupled Electron-Transfer Mechanism of Flavin-Dependent Hydroxylases. Journal of Physical Chemistry B, 2019, 123, 8065-8073.	1.2	12
90	BrÃ¸nsted-Acid-Catalyzed Intramolecular Carbonylâ€“Olefin Reactions: Interrupted Metathesis vs Carbonyl-Ene Reaction. Journal of Organic Chemistry, 2021, 86, 3008-3016.	1.7	12

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91	Investigating the Optical Properties of Thiophene Additions to s-Indacene Donors with Diketopyrrolopyrrole, Isoindigo, and Thienothiophene Acceptors. Journal of Physical Chemistry C, 2018, 122, 27713-27733.	1.5	11
92	Experimental and Theoretical Characterization of Ultrafast Water-Soluble Photochromic Photoacids. Journal of Physical Chemistry B, 2021, 125, 4120-4131.	1.2	11
93	Using Adhesives to Capture Microplastics from Water. ACS ES&T Engineering, 2021, 1, 1698-1704.	3.7	11
94	Estimating the Derivative Coupling Vector Using Gradients. Journal of Physical Chemistry Letters, 2016, 7, 5074-5079.	2.1	10
95	Uncovering reaction sequences on surfaces through graphical methods. Physical Chemistry Chemical Physics, 2018, 20, 7721-7729.	1.3	10
96	Trials and tribulations of designing multitasking catalysts for olefin/thiophene block copolymerizations. Journal of Polymer Science Part A, 2018, 56, 132-137.	2.5	10
97	Charge transfer via spin flip configuration interaction: Benchmarks and application to singlet fission. Journal of Chemical Physics, 2020, 153, 064109.	1.2	10
98	Toward Full Configuration Interaction for Transition-Metal Complexes. Journal of Physical Chemistry A, 2021, 125, 1598-1609.	1.1	10
99	Nickel-Catalyzed Three-Component Cycloadditions of Enoates, Alkynes, and Aldehydes. Journal of Organic Chemistry, 2020, 85, 2956-2965.	1.7	9
100	Mercury Magnetic Isotope Effect: A Plausible Photochemical Mechanism. Journal of Physical Chemistry A, 2020, 124, 3711-3719.	1.1	9
101	The Role of the Core Attachment Positioning in Triggering Intramolecular Singlet Exciton Fission in Perylene Diimide Tetramers. Journal of Physical Chemistry B, 2021, 125, 5114-5131.	1.2	9
102	Investigation of Thermally Activated Delayed Fluorescence in Donorâ€“Acceptor Organic Emitters with Time-Resolved Absorption Spectroscopy. Chemistry of Materials, 2022, 34, 2161-2175.	3.2	9
103	Orbitals with intermediate localization and low coupling: Spanning the gap between canonical and localized orbitals. Journal of Chemical Physics, 2015, 143, 014106.	1.2	8
104	Fully variational incremental CASSCF. Journal of Chemical Physics, 2021, 154, 014105.	1.2	8
105	Mechanochemical Release of N â€Heterocyclic Carbenes from Flexâ€Activated Mechanophores. Angewandte Chemie, 2021, 133, 13671-13675.	1.6	8
106	Studies of Catalyst-Controlled Regioselective Acetalization and Its Application to Single-Pot Synthesis of Differentially Protected Saccharides. Journal of the American Chemical Society, 2021, 143, 18592-18604.	6.6	8
107	Quantum Chemical Investigation of Dimerization in the Schlenk Equilibrium of Thiophene Grignard Reagents. Journal of Physical Chemistry A, 2020, 124, 1480-1488.	1.1	7
108	The Mechanics of the Bicycle Pedal Photoisomerization in Crystalline cis,cis-1,4-Diphenyl-1,3-butadiene. Journal of Physical Chemistry A, 2020, 124, 8897-8906.	1.1	6

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109	Combined Theoretical and Experimental Investigation of Lewis Acid-Carbonyl Interactions for Metathesis. ACS Catalysis, 2021, 11, 4381-4394.	5.5	6
110	Experimental and Computational Studies on Regiodivergent Chiral Phosphoric Acid Catalyzed Cycloisomerization of Mupirocin Methyl Ester. Chemistry - A European Journal, 2020, 26, 4583-4591.	1.7	5
111	An Ionâ€Pairing Approach to Stereoselective Metalâ€Free Ringâ€Opening Metathesis Polymerization. Angewandte Chemie, 2021, 133, 14071-14077.	1.6	5
112	Iterative submatrix diagonalisation for large configuration interaction problems. Molecular Physics, 2018, 116, 107-117.	0.8	3
113	Impact of Ring-Fusion on the Excited State Decay Pathways of N-Annulated Perylene Diimides. Journal of Physical Chemistry C, 2021, 125, 10500-10515.	1.5	3
114	An Openâ€Shell Coronoid with Hybrid Chichibabinâ€“Schlenk Conjugation. Angewandte Chemie, 2021, 133, 22670-22678.	1.6	3
115	Toward oneâ€pot olefin/thiophene block copolymers using an in situ ligand exchange. Journal of Polymer Science Part A, 2019, 57, 1601-1605.	2.5	2
116	Interplay Between Applied Force and Radical Attack in the Mechanochemical Chain Scission of Poly(acrylic acid). Journal of Physical Chemistry A, 2022, 126, 521-528.	1.1	2
117	Changes in ligand coordination mode induce bimetallic Câ€“C coupling pathways. Dalton Transactions, 2022, 51, 3977-3991.	1.6	2
118	The many-body electronic interactions of Fe(II)â€“porphyrin. Journal of Chemical Physics, 2022, 156, 094110.	1.2	2
119	Glycosyl Exchange of Unactivated Glycosidic Bonds: Suppressing or Embracing Side Reactivity in Catalytic Glycosylations. Journal of Organic Chemistry, 2022, 87, 5817-5826.	1.7	2
120	Stepwise basis set selection. Journal of Computational Chemistry, 2018, 39, 2153-2162.	1.5	1
121	Using J_{PP} to Identify Ni Bidentate Phosphine Complexes In Situ. Inorganic Chemistry, 2021, 60, 13400-13408.	1.9	1
122	State-specific solvation for restricted active space spinâ€“flip (RAS-SF) wave functions based on the polarizable continuum formalism. Journal of Chemical Physics, 2022, 156, .	1.2	1