Steven E Wheeler

List of Publications by Year
in descending order

110	7,410	57719	54882
papers	citations	44 h-index	84 g-index

138	138	138	7421
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A Hierarchy of Homodesmotic Reactions for Thermochemistry. Journal of the American Chemical Society, 2009, 131, 2547-2560.	6.6	508
2	Understanding Substituent Effects in Noncovalent Interactions Involving Aromatic Rings. Accounts of Chemical Research, 2013, 46, 1029-1038.	7.6	448
3	Substituent Effects in the Benzene Dimer are Due to Direct Interactions of the Substituents with the Unsubstituted Benzene. Journal of the American Chemical Society, 2008, 130, 10854-10855.	6.6	432
4	Local Nature of Substituent Effects in Stacking Interactions. Journal of the American Chemical Society, 2011, 133, 10262-10274.	6.6	395
5	Integration Grid Errors for Meta-GGA-Predicted Reaction Energies: Origin of Grid Errors for the M06 Suite of Functionals. Journal of Chemical Theory and Computation, 2010, 6, 395-404.	2.3	332
6	Bifurcations on Potential Energy Surfaces of Organic Reactions. Angewandte Chemie - International Edition, 2008, 47, 7592-7601.	7.2	316
7	Noncovalent Interactions in Organocatalysis and the Prospect of Computational Catalyst Design. Accounts of Chemical Research, 2016, 49, 1061-1069.	7.6	306
8	Toward a More Complete Understanding of Noncovalent Interactions Involving Aromatic Rings. Journal of Physical Chemistry A, 2014, 118, 6133-6147.	1.1	292
9	Chiral phosphoric acid catalysis: from numbers to insights. Chemical Society Reviews, 2018, 47, 1142-1158.	18.7	251
10	Through-Space Effects of Substituents Dominate Molecular Electrostatic Potentials of Substituted Arenes. Journal of Chemical Theory and Computation, 2009, 5, 2301-2312.	2.3	201
11	Substituent Effects in Cation/Ï€ Interactions and Electrostatic Potentials above the Centers of Substituted Benzenes Are Due Primarily to Through-Space Effects of the Substituents. Journal of the American Chemical Society, 2009, 131, 3126-3127.	6.6	188
12	Probing Substituent Effects in Arylâˆ’Aryl Interactions Using Stereoselective Dielsâˆ’Alder Cycloadditions. Journal of the American Chemical Society, 2010, 132, 3304-3311.	6.6	176
13	Taking the Aromaticity out of Aromatic Interactions. Angewandte Chemie - International Edition, 2011, 50, 7847-7849.	7.2	167
14	Substituent Effects on Nonâ€Covalent Interactions with Aromatic Rings: Insights from Computational Chemistry. ChemPhysChem, 2011, 12, 3116-3130.	1.0	132
15	Are Anion/Ï€ Interactions Actually a Case of Simple Chargeâˆ’Dipole Interactions?^{â€}. Journal of Physical Chemistry A, 2010, 114, 8658-8664.	1.1	131
16	Accurate Reaction Enthalpies and Sources of Error in DFT Thermochemistry for Aldol, Mannich, and Î±-Aminoxylation Reactions. Journal of Physical Chemistry A, 2009, 113, 10376-10384.	1.1	124
17	AARON: An Automated Reaction Optimizer for New Catalysts. Journal of Chemical Theory and Computation, 2018, 14, 5249-5261.	2.3	103
18	Physical Nature of Substituent Effects in XH/Ï€ Interactions. Journal of Chemical Theory and Computation, 2012, 8, 3167-3174.	2.3	89

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19	Homodesmotic reactions for thermochemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 204-220.	6.2	85
20	Ionization Thresholds of Small Carbon Clusters:â€‰ Tunable VUV Experiments and Theory. Journal of the American Chemical Society, 2007, 129, 10229-10243.	6.6	82
21	Origin of substituent effects in edge-to-face arylâ€“aryl interactions. Molecular Physics, 2009, 107, 749-760.	0.8	76
22	Low Band Gap Coplanar Conjugated Molecules Featuring Dynamic Intramolecular Lewis Acidâ€“Base Coordination. Journal of Organic Chemistry, 2016, 81, 4347-4352.	1.7	73
23	Thinking Out of the Black Box:â€‰ Accurate Barrier Heights of 1,3-Dipolar Cycloadditions of Ozone with Acetylene and Ethylene. Journal of Physical Chemistry A, 2008, 112, 1798-1807.	1.1	72
24	Enantioselectivity in Catalytic Asymmetric Fischer Indolizations Hinges on the Competition of Ï€-Stacking and CH/Ï€ Interactions. Organic Letters, 2015, 17, 3066-3069.	2.4	72
25	Predicting the Strength of Stacking Interactions between Heterocycles and Aromatic Amino Acid Side Chains. Journal of the American Chemical Society, 2019, 141, 11027-11035.	6.6	70
26	Design of Organocatalysts for Asymmetric Propargylations through Computational Screening. ACS Catalysis, 2016, 6, 7948-7955.	5.5	68
27	Thermochemistry of disputed soot formation intermediates C4H3 and C4H5. Journal of Chemical Physics, 2004, 121, 8800-8813.	1.2	66
28	Extraordinary Difference in Reactivity of Ozone (OOO) and Sulfur Dioxide (OSO): A Theoretical Study. Journal of Chemical Theory and Computation, 2011, 7, 2104-2111.	2.3	63
29	Two Rapid Catalyst-Free Click Reactions for In Vivo Protein Labeling of Genetically Encoded Strained Alkene/Alkyne Functionalities. Bioconjugate Chemistry, 2014, 25, 1730-1738.	1.8	59
30	Microsolvation effects on the electron capturing ability of thymine: Thymine-water clusters. Journal of Chemical Physics, 2006, 124, 204310.	1.2	58
31	Anionâ€“Ï€ interactions and positive electrostatic potentials of N-heterocycles arise from the positions of the nuclei, not changes in the Ï€-electron distribution. Chemical Communications, 2014, 50, 11118-11121.	2.2	58
32	Origin of Enantioselectivity in the Propargylation of Aromatic Aldehydes Catalyzed by Helical N-Oxides. Journal of the American Chemical Society, 2012, 134, 3095-3102.	6.6	57
33	Electrostatic Basis for Enantioselective BrÃ¸nsted-Acid-Catalyzed Asymmetric Ring Openings of meso-Epoxides. ACS Catalysis, 2016, 6, 2681-2688.	5.5	56
34	Thermochemistry of Key Soot Formation Intermediates:Â C3H3Isomersâ€. Journal of Physical Chemistry A, 2007, 111, 3819-3830.	1.1	55
35	Stacking and Electrostatic Interactions Drive the Stereoselectivity of Silyliumâ€Ion Asymmetric Counteranionâ€Directed Catalysis. Angewandte Chemie - International Edition, 2016, 55, 15889-15893.	7.2	55
36	Binding energies of small lithium clusters (Lin) and hydrogenated lithium clusters (LinH). Journal of Chemical Physics, 2004, 120, 4683-4689.	1.2	53

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37	Time-Resolved Surface-Enhanced Coherent Sensing of Nanoscale Molecular Complexes. Scientific Reports, 2012, 2, 891.	1.6	50
38	Measurement and Theory of Hydrogen Bonding Contribution to Isosteric DNA Base Pairs. Journal of the American Chemical Society, 2012, 134, 3154-3163.	6.6	50
39	Origin of the Superior Performance of (Thio)Squaramides over (Thio)Ureas in Organocatalysis. Chemistry - A European Journal, 2013, 19, 15141-15147.	1.7	48
40	Thermochemistry of the HOSO Radical, a Key Intermediate in Fossil Fuel Combustion. Journal of Physical Chemistry A, 2009, 113, 6779-6788.	1.1	47
41	Prospects for the Computational Design of Bipyridine N,Nâ€²-Dioxide Catalysts for Asymmetric Propargylation Reactions. ACS Catalysis, 2015, 5, 272-280.	5.5	46
42	Enantioselective Synthesis of Chiral Oxime Ethers: Desymmetrization and Dynamic Kinetic Resolution of Substituted Cyclohexanones. Angewandte Chemie - International Edition, 2017, 56, 2454-2458.	7.2	46
43	Activation Mode and Origin of Selectivity in Chiral Phosphoric Acid-Catalyzed Oxacycle Formation by Intramolecular Oxetane Desymmetrizations. ACS Catalysis, 2017, 7, 7332-7339.	5.5	45
44	Automated Quantum Mechanical Predictions of Enantioselectivity in a Rhodiumâ€Catalyzed Asymmetric Hydrogenation. Angewandte Chemie - International Edition, 2017, 56, 9101-9105.	7.2	43
45	Quantifying the Role of Anionâ^Ï€ Interactions in Anionâ^Ï€ Catalysis. Organic Letters, 2014, 16, 3268-3271.	2.4	42
46	Benchmark Torsional Potentials of Building Blocks for Conjugated Materials: Bifuran, Bithiophene, and Biselenophene. Journal of Chemical Theory and Computation, 2014, 10, 3647-3655.	2.3	41
47	Competing Noncovalent Interactions Control the Stereoselectivity of Chiral Phosphoric Acid Catalyzed Ring Openings of 3-Substituted Oxetanes. ACS Catalysis, 2016, 6, 7222-7228.	5.5	41
48	Molecular Coplanarity and Self-Assembly Promoted by Intramolecular Hydrogen Bonds. Organic Letters, 2016, 18, 6332-6335.	2.4	39
49	Importance of Electrostatic Effects in the Stereoselectivity of NHC-Catalyzed Kinetic Resolutions. Journal of the American Chemical Society, 2017, 139, 12441-12449.	6.6	39
50	The deprotonated guanine-cytosine base pair. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 7554-7559.	3.3	38
51	Accelerating Ni(ii) precatalyst initiation using reactive ligands and its impact on chain-growth polymerizations. Dalton Transactions, 2013, 42, 4218.	1.6	37
52	Broad Transferability of Substituent Effects in Ï€-Stacking Interactions Provides New Insights into Their Origin. Journal of Chemical Theory and Computation, 2013, 9, 3479-3490.	2.3	37
53	Noncovalent Interactions of a Benzo[a]pyrene Diol Epoxide with DNA Base Pairs: Insight into the Formation of Adducts of (+)-BaP DE-2 with DNA. Journal of Physical Chemistry A, 2010, 114, 2038-2044.	1.1	33
54	Accurate Thermochemistry of Hydrocarbon Radicals via an Extended Generalized Bond Separation Reaction Scheme. Journal of Physical Chemistry A, 2012, 116, 3436-3447.	1.1	33

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55	Quantifying the Ï€-Stacking Interactions in Nitroarene Binding Sites of Proteins. Journal of Physical Chemistry B, 2015, 119, 14441-14450.	1.2	30
56	Torsional Barriers to Rotation and Planarization in Heterocyclic Oligomers of Value in Organic Electronics. Journal of Chemical Theory and Computation, 2017, 13, 5624-5638.	2.3	30
57	Explaining the Disparate Stereoselectivities of N-Oxide Catalyzed Allylations and Propargylations of Aldehydes. Organic Letters, 2012, 14, 5310-5313.	2.4	28
58	<scp>QChASM</scp>: Quantum chemistry automation and structure manipulation. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1510.	6.2	28
59	Stacking Interactions of Heterocyclic Drug Fragments with Protein Amide Backbones. ChemMedChem, 2018, 13, 835-841.	1.6	26
60	Controlling the local arrangements of Ï€-stacked polycyclic aromatic hydrocarbons through substituent effects. CrystEngComm, 2012, 14, 6140.	1.3	25
61	On the nature of the MÃ¸ller-Plesset critical point. Journal of Chemical Physics, 2005, 123, 064105.	1.2	24
62	Macrocycle Embrace: Encapsulation of Fluoroarenes by mâ€Phenylene Ethynylene Host. Chemistry - A European Journal, 2015, 21, 2750-2754.	1.7	24
63	Electron affinities of the radicals derived from cytosine. Physical Chemistry Chemical Physics, 2005, 7, 861.	1.3	23
64	Impact of Neighboring Chains on Torsional Defects in Oligothiophenes. Journal of Physical Chemistry A, 2012, 116, 2997-3003.	1.1	23
65	Endohedral and exohedral complexes of substituted benzenes with carbon nanotubes and graphene. Journal of Chemical Physics, 2013, 139, 094703.	1.2	22
66	Stacking Interactions between 9-Methyladenine and Heterocycles Commonly Found in Pharmaceuticals. Journal of Chemical Information and Modeling, 2016, 56, 906-914.	2.5	22
67	Ionization potentials of small lithium clusters (Lin) and hydrogenated lithium clusters (LinH). Journal of Chemical Physics, 2005, 122, 204328.	1.2	21
68	Anion-Ï€ Interactions in Computer-Aided Drug Design: Modeling the Inhibition of Malate Synthase by Phenyl-Diketo Acids. Journal of Chemical Information and Modeling, 2018, 58, 2085-2091.	2.5	21
69	Remarkable electron accepting properties of the simplest benzenoid cyanocarbons: hexacyanobenzene, octacyanonaphthalene and decacyanoanthracene. Chemical Communications, 2006, , 758.	2.2	20
70	Harnessing weak interactions for enantioselective catalysis. Science, 2015, 347, 719-720.	6.0	20
71	Ring-Walking of Zerovalent Nickel on Aryl Halides. Journal of Chemical Theory and Computation, 2017, 13, 1706-1711.	2.3	19
72	SASS: A symmetry adapted stochastic search algorithm exploiting site symmetry. Journal of Chemical Physics, 2007, 126, 104104.	1.2	18

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73	Performance of DFT methods and origin of stereoselectivity in bipyridine N,Nâ€²-dioxide catalyzed allylation and propargylation reactions. Organic and Biomolecular Chemistry, 2014, 12, 8346-8353.	1.5	18
74	Biomimetic Total Syntheses of (â˜)â€Leucoridinesâ€…A and C through the Dimerization of (â˜)â€Dihydrovalparicine. Angewandte Chemie - International Edition, 2015, 54, 12632-12635.	7.2	17
75	Conformational behavior and stacking interactions of contorted polycyclic aromatics. Physical Chemistry Chemical Physics, 2017, 19, 18186-18193.	1.3	17
76	Tuning Stacking Interactions between Aspâ€“Arg Salt Bridges and Heterocyclic Drug Fragments. Journal of Chemical Information and Modeling, 2019, 59, 149-158.	2.5	17
77	Modulating Stereoselectivity through Electrostatic Interactions in a SPINOL-Phosphoric Acid-Catalyzed Synthesis of 2,3-Dihydroquinazolinones. ACS Catalysis, 2020, 10, 12292-12299.	5.5	17
78	The Pentacyanocyclopentadienyl System:Â Structures and Energetics. Journal of Physical Chemistry A, 2005, 109, 10084-10091.	1.1	16
79	Revised Role of Selectfluor in Homogeneous Auâ€Catalyzed Oxidative Cï£¿O Bond Formations. Chemistry - A European Journal, 2014, 20, 15833-15839.	1.7	16
80	On the convergence of Z-averaged perturbation theory. Journal of Chemical Physics, 2008, 128, 074107.	1.2	15
81	Stacked homodimers of substituted contorted hexabenzocoronenes and their complexes with C₆₀ fullerene. Organic and Biomolecular Chemistry, 2017, 15, 6042-6049.	1.5	14
82	<scp>SEQCROW</scp>: A<scp>ChimeraX</scp>bundle to facilitate quantum chemical applications to complex molecular systems. Journal of Computational Chemistry, 2021, 42, 1750-1754.	1.5	14
83	Protonated carbonyl sulfide: Prospects for the spectroscopic observation of the elusive HSCO+ isomer. Journal of Chemical Physics, 2006, 124, 044322.	1.2	13
84	The Vinyl Radical and Fluorinated Vinyl Radicals, C2H3-nFn (n = 0â˜3), and Corresponding Anions:â€‰ Comparison with the Isoelectronic Complexes [XÂ·Â·Â·YCâ‰¡CZ]-. Journal of Physical Chemistry A, 2004, 108, 1608-1615.	1.1	12
85	Aromatic Interactions Modulate the 5â€²-Base Selectivity of the DNA-Binding Autoantibody ED-10. Journal of Physical Chemistry B, 2014, 118, 5653-5659.	1.2	12
86	Stacking and Electrostatic Interactions Drive the Stereoselectivity of Silyliumâ€Ion Asymmetric Counteranionâ€Directed Catalysis. Angewandte Chemie, 2016, 128, 16121-16125.	1.6	11
87	Enantioselective Synthesis of Chiral Oxime Ethers: Desymmetrization and Dynamic Kinetic Resolution of Substituted Cyclohexanones. Angewandte Chemie, 2017, 129, 2494-2498.	1.6	11
88	Reactive ligand influence on initiation in phenylene catalystâ€transfer polymerization. Journal of Polymer Science Part A, 2017, 55, 1530-1535.	2.5	11
89	Converting SMILES to Stacking Interaction Energies. Journal of Chemical Information and Modeling, 2019, 59, 3413-3421.	2.5	11
90	Understanding the Reactivity and Selectivity of Fluxional Chiral DMAPâ€Catalyzed Kinetic Resolutions of Axially Chiral Biaryls. Chemistry - A European Journal, 2019, 25, 4452-4459.	1.7	11

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91	Hydrogen-Abstracted Adenineâ˜Thymine Radicals with Interesting Transferable Properties. Journal of Physical Chemistry B, 2007, 111, 5525-5530.	1.2	10
92	Vibrational Spectroscopy and Theory of the Protonated Benzene Dimer and Trimer. Journal of Physical Chemistry A, 2012, 116, 7065-7073.	1.1	10
93	Optimization of Catalyst Structure for Asymmetric Propargylation of Aldehydes with Allenyltrichlorosilane. Advanced Synthesis and Catalysis, 2020, 362, 5467-5474.	2.1	10
94	Intercolumnar Interactions Control the Local Orientations within Columnar Stacks of Sumanene and Sumanene Derivatives. Journal of Physical Chemistry C, 2017, 121, 8541-8547.	1.5	9
95	Lone-Pair-Induced Topicity Observed in Macrobicyclic Tetra-thia Lactams and Cryptands: Synthesis, Spectral Identification, and Computational Assessment. Journal of Organic Chemistry, 2018, 83, 10025-10036.	1.7	7
96	Better Sensing through Stacking: The Role of Non-Covalent Interactions in Guanine-Binding Sensors. Journal of Physical Chemistry B, 2019, 123, 487-495.	1.2	7
97	The extremely flat torsional potential energy surface of oxalyl chloride. Journal of Chemical Physics, 2005, 122, 234313.	1.2	6
98	Reply to â€œComment on â€˜Accurate Thermochemistry of Hydrocarbon Radicals via an Extended Generalized Bond Separation Reaction Schemeâ€™â€• Journal of Physical Chemistry A, 2012, 116, 8794-8796.	1.1	6
99	Rennerâ˜Teller Bending Frequencies of the Ãƒ 2Î State of OCS+. Journal of Physical Chemistry A, 2007, 111, 4551-4555.	1.1	5
100	Automated Quantum Mechanical Predictions of Enantioselectivity in a Rhodiumâ€Catalyzed Asymmetric Hydrogenation. Angewandte Chemie, 2017, 129, 9229-9233.	1.6	5
101	Topomeric aza/thia cryptands: synthesis and theoretical aspects of in/out isomerism using n-alkyl bridging. Organic Chemistry Frontiers, 2020, 7, 1164-1176.	2.3	5
102	Importance of favourable non-covalent contacts in the stereoselective synthesis of tetrasubstituted chromanones. Organic Chemistry Frontiers, 2022, 9, 3027-3033.	2.3	5
103	Importance of model size in quantum mechanical studies of DNA intercalation. Journal of Computational Chemistry, 2020, 41, 1175-1184.	1.5	4
104	Mechanism and Origin of Selectivity in Platinum(II)â€Catalyzed Reactions of Acyclic Î³,Î´â€Ynones with Alkenes. ChemCatChem, 2016, 8, 2771-2780.	1.8	3
105	Weak Intermolecular Interactions. , 2018, , 289-319.		3
106	Synthesis, Biological Evaluation, and Computational Analysis of Biaryl Sideâ€Chain Analogs of Solithromycin. ChemMedChem, 2021, 16, 3368-3373.	1.6	3
107	Unraveling the Origin of Substituents Effects in Ï€-Stacking Interactions. Challenges and Advances in Computational Chemistry and Physics, 2015, , 421-442.	0.6	2
108	Solvent dependence of the stereoselectivity in bipyridine N,Nâ€²-dioxide catalyzed allylation of aromatic aldehydes: A computational perspective. Molecular Catalysis, 2020, 483, 110712.	1.0	2

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109	Theoretical study on the origin of enantioselectivity in the primary amineâ€“BrÃ¸nsted acid catalyzed epoxidation of cyclic enones. Tetrahedron: Asymmetry, 2013, 24, 1598-1604.	1.8	1
110	Crystal engineering of heterocyclic arylene(ethynylene) oligomers through programmed aromatic stacking. Journal of Materials Chemistry C, 0, , .	2.7	1