Steven E Wheeler

List of Publications by Year
in descending order

110	7,410	57758	54911
papers	citations	44 h-index	84 g-index

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

#	Article	IF	Citations
1	Importance of favourable non-covalent contacts in the stereoselective synthesis of tetrasubstituted chromanones. Organic Chemistry Frontiers, 2022, 9, 3027-3033.	4.5	5
2	<scp>QChASM</scp>: Quantum chemistry automation and structure manipulation. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1510.	14.6	28
3	<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.	3.3	14
4	Synthesis, Biological Evaluation, and Computational Analysis of Biaryl Sideâ€Chain Analogs of Solithromycin. ChemMedChem, 2021, 16, 3368-3373.	3.2	3
5	Solvent dependence of the stereoselectivity in bipyridine N,Nâ€²-dioxide catalyzed allylation of aromatic aldehydes: A computational perspective. Molecular Catalysis, 2020, 483, 110712.	2.0	2
6	Optimization of Catalyst Structure for Asymmetric Propargylation of Aldehydes with Allenyltrichlorosilane. Advanced Synthesis and Catalysis, 2020, 362, 5467-5474.	4.3	10
7	Modulating Stereoselectivity through Electrostatic Interactions in a SPINOL-Phosphoric Acid-Catalyzed Synthesis of 2,3-Dihydroquinazolinones. ACS Catalysis, 2020, 10, 12292-12299.	11.2	17
8	Topomeric aza/thia cryptands: synthesis and theoretical aspects of in/out isomerism using n-alkyl bridging. Organic Chemistry Frontiers, 2020, 7, 1164-1176.	4.5	5
9	Importance of model size in quantum mechanical studies of DNA intercalation. Journal of Computational Chemistry, 2020, 41, 1175-1184.	3.3	4
10	Converting SMILES to Stacking Interaction Energies. Journal of Chemical Information and Modeling, 2019, 59, 3413-3421.	5.4	11
11	Predicting the Strength of Stacking Interactions between Heterocycles and Aromatic Amino Acid Side Chains. Journal of the American Chemical Society, 2019, 141, 11027-11035.	13.7	70
12	Better Sensing through Stacking: The Role of Non-Covalent Interactions in Guanine-Binding Sensors. Journal of Physical Chemistry B, 2019, 123, 487-495.	2.6	7
13	Understanding the Reactivity and Selectivity of Fluxional Chiral DMAPâ€Catalyzed Kinetic Resolutions of Axially Chiral Biaryls. Chemistry - A European Journal, 2019, 25, 4452-4459.	3.3	11
14	Tuning Stacking Interactions between Aspâ€“Arg Salt Bridges and Heterocyclic Drug Fragments. Journal of Chemical Information and Modeling, 2019, 59, 149-158.	5.4	17
15	Weak Intermolecular Interactions. , 2018, , 289-319.		3
16	Stacking Interactions of Heterocyclic Drug Fragments with Protein Amide Backbones. ChemMedChem, 2018, 13, 835-841.	3.2	26
17	Chiral phosphoric acid catalysis: from numbers to insights. Chemical Society Reviews, 2018, 47, 1142-1158.	38.1	251
18	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.	3.2	7

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19	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.	5.4	21
20	AARON: An Automated Reaction Optimizer for New Catalysts. Journal of Chemical Theory and Computation, 2018, 14, 5249-5261.	5.3	103
21	Enantioselective Synthesis of Chiral Oxime Ethers: Desymmetrization and Dynamic Kinetic Resolution of Substituted Cyclohexanones. Angewandte Chemie, 2017, 129, 2494-2498.	2.0	11
22	Enantioselective Synthesis of Chiral Oxime Ethers: Desymmetrization and Dynamic Kinetic Resolution of Substituted Cyclohexanones. Angewandte Chemie - International Edition, 2017, 56, 2454-2458.	13.8	46
23	Ring-Walking of Zerovalent Nickel on Aryl Halides. Journal of Chemical Theory and Computation, 2017, 13, 1706-1711.	5.3	19
24	Reactive ligand influence on initiation in phenylene catalystâ€transfer polymerization. Journal of Polymer Science Part A, 2017, 55, 1530-1535.	2.3	11
25	Conformational behavior and stacking interactions of contorted polycyclic aromatics. Physical Chemistry Chemical Physics, 2017, 19, 18186-18193.	2.8	17
26	Stacked homodimers of substituted contorted hexabenzocoronenes and their complexes with C₆₀ fullerene. Organic and Biomolecular Chemistry, 2017, 15, 6042-6049.	2.8	14
27	Automated Quantum Mechanical Predictions of Enantioselectivity in a Rhodiumâ€Catalyzed Asymmetric Hydrogenation. Angewandte Chemie, 2017, 129, 9229-9233.	2.0	5
28	Automated Quantum Mechanical Predictions of Enantioselectivity in a Rhodiumâ€Catalyzed Asymmetric Hydrogenation. Angewandte Chemie - International Edition, 2017, 56, 9101-9105.	13.8	43
29	Intercolumnar Interactions Control the Local Orientations within Columnar Stacks of Sumanene and Sumanene Derivatives. Journal of Physical Chemistry C, 2017, 121, 8541-8547.	3.1	9
30	Torsional Barriers to Rotation and Planarization in Heterocyclic Oligomers of Value in Organic Electronics. Journal of Chemical Theory and Computation, 2017, 13, 5624-5638.	5.3	30
31	Activation Mode and Origin of Selectivity in Chiral Phosphoric Acid-Catalyzed Oxacycle Formation by Intramolecular Oxetane Desymmetrizations. ACS Catalysis, 2017, 7, 7332-7339.	11.2	45
32	Importance of Electrostatic Effects in the Stereoselectivity of NHC-Catalyzed Kinetic Resolutions. Journal of the American Chemical Society, 2017, 139, 12441-12449.	13.7	39
33	Stacking and Electrostatic Interactions Drive the Stereoselectivity of Silyliumâ€Ion Asymmetric Counteranionâ€Directed Catalysis. Angewandte Chemie, 2016, 128, 16121-16125.	2.0	11
34	Molecular Coplanarity and Self-Assembly Promoted by Intramolecular Hydrogen Bonds. Organic Letters, 2016, 18, 6332-6335.	4.6	39
35	Noncovalent Interactions in Organocatalysis and the Prospect of Computational Catalyst Design. Accounts of Chemical Research, 2016, 49, 1061-1069.	15.6	306
36	Stacking Interactions between 9-Methyladenine and Heterocycles Commonly Found in Pharmaceuticals. Journal of Chemical Information and Modeling, 2016, 56, 906-914.	5.4	22

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37	Low Band Gap Coplanar Conjugated Molecules Featuring Dynamic Intramolecular Lewis Acidâ€“Base Coordination. Journal of Organic Chemistry, 2016, 81, 4347-4352.	3.2	73
38	Mechanism and Origin of Selectivity in Platinum(II)â€Catalyzed Reactions of Acyclic Î³,Îˆâ€Ynones with Alkenes. ChemCatChem, 2016, 8, 2771-2780.	3.7	3
39	Competing Noncovalent Interactions Control the Stereoselectivity of Chiral Phosphoric Acid Catalyzed Ring Openings of 3-Substituted Oxetanes. ACS Catalysis, 2016, 6, 7222-7228.	11.2	41
40	Design of Organocatalysts for Asymmetric Propargylations through Computational Screening. ACS Catalysis, 2016, 6, 7948-7955.	11.2	68
41	Stacking and Electrostatic Interactions Drive the Stereoselectivity of Silyliumâ€Ion Asymmetric Counteranionâ€Directed Catalysis. Angewandte Chemie - International Edition, 2016, 55, 15889-15893.	13.8	55
42	Electrostatic Basis for Enantioselective BrÃ¸nsted-Acid-Catalyzed Asymmetric Ring Openings of meso-Epoxides. ACS Catalysis, 2016, 6, 2681-2688.	11.2	56
43	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.	13.8	17
44	Enantioselectivity in Catalytic Asymmetric Fischer Indolizations Hinges on the Competition of Ï€-Stacking and CH/Ï€ Interactions. Organic Letters, 2015, 17, 3066-3069.	4.6	72
45	Harnessing weak interactions for enantioselective catalysis. Science, 2015, 347, 719-720.	12.6	20
46	Unraveling the Origin of Substituents Effects in Ï€-Stacking Interactions. Challenges and Advances in Computational Chemistry and Physics, 2015, , 421-442.	0.6	2
47	Quantifying the Ï€-Stacking Interactions in Nitroarene Binding Sites of Proteins. Journal of Physical Chemistry B, 2015, 119, 14441-14450.	2.6	30
48	Prospects for the Computational Design of Bipyridine N,Nâ€²-Dioxide Catalysts for Asymmetric Propargylation Reactions. ACS Catalysis, 2015, 5, 272-280.	11.2	46
49	Macrocycle Embrace: Encapsulation of Fluoroarenes by mâ€Phenylene Ethynylene Host. Chemistry - A European Journal, 2015, 21, 2750-2754.	3.3	24
50	Aromatic Interactions Modulate the 5â€²-Base Selectivity of the DNA-Binding Autoantibody ED-10. Journal of Physical Chemistry B, 2014, 118, 5653-5659.	2.6	12
51	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.	4.1	58
52	Revised Role of Selectfluor in Homogeneous Auâ€Catalyzed Oxidative Cï£¿O Bond Formations. Chemistry - A European Journal, 2014, 20, 15833-15839.	3.3	16
53	Two Rapid Catalyst-Free Click Reactions for In Vivo Protein Labeling of Genetically Encoded Strained Alkene/Alkyne Functionalities. Bioconjugate Chemistry, 2014, 25, 1730-1738.	3.6	59
54	Benchmark Torsional Potentials of Building Blocks for Conjugated Materials: Bifuran, Bithiophene, and Biselenophene. Journal of Chemical Theory and Computation, 2014, 10, 3647-3655.	5.3	41

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55	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.	2.8	18
56	Quantifying the Role of Anionâˆ’Ï€ Interactions in Anionâˆ’Ï€ Catalysis. Organic Letters, 2014, 16, 3268-3271.	4.6	42
57	Toward a More Complete Understanding of Noncovalent Interactions Involving Aromatic Rings. Journal of Physical Chemistry A, 2014, 118, 6133-6147.	2.5	292
58	Understanding Substituent Effects in Noncovalent Interactions Involving Aromatic Rings. Accounts of Chemical Research, 2013, 46, 1029-1038.	15.6	448
59	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
60	Endohedral and exohedral complexes of substituted benzenes with carbon nanotubes and graphene. Journal of Chemical Physics, 2013, 139, 094703.	3.0	22
61	Accelerating Ni(ii) precatalyst initiation using reactive ligands and its impact on chain-growth polymerizations. Dalton Transactions, 2013, 42, 4218.	3.3	37
62	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.	5.3	37
63	Origin of the Superior Performance of (Thio)Squaramides over (Thio)Ureas in Organocatalysis. Chemistry - A European Journal, 2013, 19, 15141-15147.	3.3	48
64	Time-Resolved Surface-Enhanced Coherent Sensing of Nanoscale Molecular Complexes. Scientific Reports, 2012, 2, 891.	3.3	50
65	Accurate Thermochemistry of Hydrocarbon Radicals via an Extended Generalized Bond Separation Reaction Scheme. Journal of Physical Chemistry A, 2012, 116, 3436-3447.	2.5	33
66	Explaining the Disparate Stereoselectivities of N-Oxide Catalyzed Allylations and Propargylations of Aldehydes. Organic Letters, 2012, 14, 5310-5313.	4.6	28
67	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.	2.5	6
68	Physical Nature of Substituent Effects in XH/Ï€ Interactions. Journal of Chemical Theory and Computation, 2012, 8, 3167-3174.	5.3	89
69	Vibrational Spectroscopy and Theory of the Protonated Benzene Dimer and Trimer. Journal of Physical Chemistry A, 2012, 116, 7065-7073.	2.5	10
70	Controlling the local arrangements of Ï€-stacked polycyclic aromatic hydrocarbons through substituent effects. CrystEngComm, 2012, 14, 6140.	2.6	25
71	Origin of Enantioselectivity in the Propargylation of Aromatic Aldehydes Catalyzed by Helical N-Oxides. Journal of the American Chemical Society, 2012, 134, 3095-3102.	13.7	57
72	Homodesmotic reactions for thermochemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 204-220.	14.6	85

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73	Measurement and Theory of Hydrogen Bonding Contribution to Isosteric DNA Base Pairs. Journal of the American Chemical Society, 2012, 134, 3154-3163.	13.7	50
74	Impact of Neighboring Chains on Torsional Defects in Oligothiophenes. Journal of Physical Chemistry A, 2012, 116, 2997-3003.	2.5	23
75	Extraordinary Difference in Reactivity of Ozone (OOO) and Sulfur Dioxide (OSO): A Theoretical Study. Journal of Chemical Theory and Computation, 2011, 7, 2104-2111.	5.3	63
76	Local Nature of Substituent Effects in Stacking Interactions. Journal of the American Chemical Society, 2011, 133, 10262-10274.	13.7	395
77	Substituent Effects on Nonâ€Covalent Interactions with Aromatic Rings: Insights from Computational Chemistry. ChemPhysChem, 2011, 12, 3116-3130.	2.1	132
78	Taking the Aromaticity out of Aromatic Interactions. Angewandte Chemie - International Edition, 2011, 50, 7847-7849.	13.8	167
79	Probing Substituent Effects in Arylâ^'Aryl Interactions Using Stereoselective Dielsâ^'Alder Cycloadditions. Journal of the American Chemical Society, 2010, 132, 3304-3311.	13.7	176
80	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.	5.3	332
81	Are Anion/Ï€ Interactions Actually a Case of Simple Chargeâ^'Dipole Interactions?^{â€}. Journal of Physical Chemistry A, 2010, 114, 8658-8664.	2.5	131
82	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.	2.5	33
83	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.	2.5	124
84	Thermochemistry of the HOSO Radical, a Key Intermediate in Fossil Fuel Combustion. Journal of Physical Chemistry A, 2009, 113, 6779-6788.	2.5	47
85	Origin of substituent effects in edge-to-face arylâ€“aryl interactions. Molecular Physics, 2009, 107, 749-760.	1.7	76
86	Through-Space Effects of Substituents Dominate Molecular Electrostatic Potentials of Substituted Arenes. Journal of Chemical Theory and Computation, 2009, 5, 2301-2312.	5.3	201
87	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.	13.7	188
88	A Hierarchy of Homodesmotic Reactions for Thermochemistry. Journal of the American Chemical Society, 2009, 131, 2547-2560.	13.7	508
89	Bifurcations on Potential Energy Surfaces of Organic Reactions. Angewandte Chemie - International Edition, 2008, 47, 7592-7601.	13.8	316
90	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.	13.7	432

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91	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.	2.5	72
92	On the convergence of Z-averaged perturbation theory. Journal of Chemical Physics, 2008, 128, 074107.	3.0	15
93	SASS: A symmetry adapted stochastic search algorithm exploiting site symmetry. Journal of Chemical Physics, 2007, 126, 104104.	3.0	18
94	Thermochemistry of Key Soot Formation Intermediates:Â C3H3Isomersâ€. Journal of Physical Chemistry A, 2007, 111, 3819-3830.	2.5	55
95	Rennerâ^'Teller Bending Frequencies of the Ãƒ 2Î State of OCS+. Journal of Physical Chemistry A, 2007, 111, 4551-4555.	2.5	5
96	Ionization Thresholds of Small Carbon Clusters:â€‰ Tunable VUV Experiments and Theory. Journal of the American Chemical Society, 2007, 129, 10229-10243.	13.7	82
97	Hydrogen-Abstracted Adenineâ^'Thymine Radicals with Interesting Transferable Properties. Journal of Physical Chemistry B, 2007, 111, 5525-5530.	2.6	10
98	Microsolvation effects on the electron capturing ability of thymine: Thymine-water clusters. Journal of Chemical Physics, 2006, 124, 204310.	3.0	58
99	Remarkable electron accepting properties of the simplest benzenoid cyanocarbons: hexacyanobenzene, octacyanonaphthalene and decacyanoanthracene. Chemical Communications, 2006, , 758.	4.1	20
100	Protonated carbonyl sulfide: Prospects for the spectroscopic observation of the elusive HSCO+ isomer. Journal of Chemical Physics, 2006, 124, 044322.	3.0	13
101	The deprotonated guanine-cytosine base pair. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 7554-7559.	7.1	38
102	The extremely flat torsional potential energy surface of oxalyl chloride. Journal of Chemical Physics, 2005, 122, 234313.	3.0	6
103	Ionization potentials of small lithium clusters (Lin) and hydrogenated lithium clusters (LinH). Journal of Chemical Physics, 2005, 122, 204328.	3.0	21
104	On the nature of the MÃ¸ller-Plesset critical point. Journal of Chemical Physics, 2005, 123, 064105.	3.0	24
105	Electron affinities of the radicals derived from cytosine. Physical Chemistry Chemical Physics, 2005, 7, 861.	2.8	23
106	The Pentacyanocyclopentadienyl System:Â Structures and Energetics. Journal of Physical Chemistry A, 2005, 109, 10084-10091.	2.5	16
107	Thermochemistry of disputed soot formation intermediates C4H3 and C4H5. Journal of Chemical Physics, 2004, 121, 8800-8813.	3.0	66
108	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.	2.5	12

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109	Binding energies of small lithium clusters (Lin) and hydrogenated lithium clusters (LinH). Journal of Chemical Physics, 2004, 120, 4683-4689.	3.0	53
110	Crystal engineering of heterocyclic arylene(ethynylene) oligomers through programmed aromatic stacking. Journal of Materials Chemistry C, 0, , .	5.5	1