# 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 | A Hierarchy of Homodesmotic Reactions for Thermochemistry. Journal of the American Chemical Society, 2009, 131, 2547-2560. | 13.7 | 508 |
| 2 | Understanding Substituent Effects in Noncovalent Interactions Involving Aromatic Rings. Accounts of Chemical Research, 2013, 46, 1029-1038. | 15.6 | 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. | 13.7 | 432 |
| 4 | Local Nature of Substituent Effects in Stacking Interactions. Journal of the American Chemical Society, 2011, 133, 10262-10274. | 13.7 | 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. | 5.3 | 332 |
| 6 | Bifurcations on Potential Energy Surfaces of Organic Reactions. Angewandte Chemie - International Edition, 2008, 47, 7592-7601. | 13.8 | 316 |
| 7 | Noncovalent Interactions in Organocatalysis and the Prospect of Computational Catalyst Design. Accounts of Chemical Research, 2016, 49, 1061-1069. | 15.6 | 306 |
| 8 | Toward a More Complete Understanding of Noncovalent Interactions Involving Aromatic Rings. Journal of Physical Chemistry A, 2014, 118, 6133-6147. | 2.5 | 292 |
| 9 | Chiral phosphoric acid catalysis: from numbers to insights. Chemical Society Reviews, 2018, 47, 1142-1158. | 38.1 | 251 |
| 10 | 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 |
| 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. | 13.7 | 188 |
| 12 | 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 |
| 13 | Taking the Aromaticity out of Aromatic Interactions. Angewandte Chemie - International Edition, 2011, 50, 7847-7849. | 13.8 | 167 |
| 14 | Substituent Effects on Nonâ€Covalent Interactions with Aromatic Rings: Insights from Computational Chemistry. ChemPhysChem, 2011, 12, 3116-3130. | 2.1 | 132 |
| 15 | Are Anion/Ï€ Interactions Actually a Case of Simple Chargeâ^'Dipole Interactions?<sup>â€</sup>. Journal of Physical Chemistry A, 2010, 114, 8658-8664. | 2.5 | 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. | 2.5 | 124 |
| 17 | AARON: An Automated Reaction Optimizer for New Catalysts. Journal of Chemical Theory and Computation, 2018, 14, 5249-5261. | 5.3 | 103 |
| 18 | Physical Nature of Substituent Effects in XH/Ï€ Interactions. Journal of Chemical Theory and Computation, 2012, 8, 3167-3174. | 5.3 | 89 |

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|---|---|---|---|
| 19 | Homodesmotic reactions for thermochemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 204-220. | 14.6 | 85 |
| 20 | 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 |
| 21 | Origin of substituent effects in edge-to-face arylâ€“aryl interactions. Molecular Physics, 2009, 107, 749-760. | 1.7 | 76 |
| 22 | Low Band Gap Coplanar Conjugated Molecules Featuring Dynamic Intramolecular Lewis Acidâ€“Base Coordination. Journal of Organic Chemistry, 2016, 81, 4347-4352. | 3.2 | 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. | 2.5 | 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. | 4.6 | 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. | 13.7 | 70 |
| 26 | Design of Organocatalysts for Asymmetric Propargylations through Computational Screening. ACS Catalysis, 2016, 6, 7948-7955. | 11.2 | 68 |
| 27 | Thermochemistry of disputed soot formation intermediates C4H3 and C4H5. Journal of Chemical Physics, 2004, 121, 8800-8813. | 3.0 | 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. | 5.3 | 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. | 3.6 | 59 |
| 30 | Microsolvation effects on the electron capturing ability of thymine: Thymine-water clusters. Journal of Chemical Physics, 2006, 124, 204310. | 3.0 | 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. | 4.1 | 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. | 13.7 | 57 |
| 33 | Electrostatic Basis for Enantioselective BrÃ¸nsted-Acid-Catalyzed Asymmetric Ring Openings of meso-Epoxides. ACS Catalysis, 2016, 6, 2681-2688. | 11.2 | 56 |
| 34 | Thermochemistry of Key Soot Formation Intermediates:Â C3H3Isomersâ€. Journal of Physical Chemistry A, 2007, 111, 3819-3830. | 2.5 | 55 |
| 35 | 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 |
| 36 | Binding energies of small lithium clusters (Lin) and hydrogenated lithium clusters (LinH). Journal of Chemical Physics, 2004, 120, 4683-4689. | 3.0 | 53 |

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| 37 | Time-Resolved Surface-Enhanced Coherent Sensing of Nanoscale Molecular Complexes. Scientific Reports, 2012, 2, 891. | 3.3 | 50 |
| 38 | 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 |
| 39 | Origin of the Superior Performance of (Thio)Squaramides over (Thio)Ureas in Organocatalysis. Chemistry - A European Journal, 2013, 19, 15141-15147. | 3.3 | 48 |
| 40 | Thermochemistry of the HOSO Radical, a Key Intermediate in Fossil Fuel Combustion. Journal of Physical Chemistry A, 2009, 113, 6779-6788. | 2.5 | 47 |
| 41 | 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 |
| 42 | 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 |
| 43 | 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 |
| 44 | Automated Quantum Mechanical Predictions of Enantioselectivity in a Rhodiumâ€Catalyzed Asymmetric Hydrogenation. Angewandte Chemie - International Edition, 2017, 56, 9101-9105. | 13.8 | 43 |
| 45 | Quantifying the Role of Anionâ^Ï€ Interactions in Anionâ^Ï€ Catalysis. Organic Letters, 2014, 16, 3268-3271. | 4.6 | 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. | 5.3 | 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. | 11.2 | 41 |
| 48 | Molecular Coplanarity and Self-Assembly Promoted by Intramolecular Hydrogen Bonds. Organic Letters, 2016, 18, 6332-6335. | 4.6 | 39 |
| 49 | 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 |
| 50 | 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 |
| 51 | Accelerating Ni(ii) precatalyst initiation using reactive ligands and its impact on chain-growth polymerizations. Dalton Transactions, 2013, 42, 4218. | 3.3 | 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. | 5.3 | 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. | 2.5 | 33 |
| 54 | 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 |

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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. | 2.6 | 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. | 5.3 | 30 |
| 57 | Explaining the Disparate Stereoselectivities of N-Oxide Catalyzed Allylations and Propargylations of Aldehydes. Organic Letters, 2012, 14, 5310-5313. | 4.6 | 28 |
| 58 | <scp>QChASM</scp>: Quantum chemistry automation and structure manipulation. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1510. | 14.6 | 28 |
| 59 | Stacking Interactions of Heterocyclic Drug Fragments with Protein Amide Backbones. ChemMedChem, 2018, 13, 835-841. | 3.2 | 26 |
| 60 | Controlling the local arrangements of Ï€-stacked polycyclic aromatic hydrocarbons through substituent effects. CrystEngComm, 2012, 14, 6140. | 2.6 | 25 |
| 61 | On the nature of the MÃ¸ller-Plesset critical point. Journal of Chemical Physics, 2005, 123, 064105. | 3.0 | 24 |
| 62 | Macrocycle Embrace: Encapsulation of Fluoroarenes by mâ€Phenylene Ethynylene Host. Chemistry - A European Journal, 2015, 21, 2750-2754. | 3.3 | 24 |
| 63 | Electron affinities of the radicals derived from cytosine. Physical Chemistry Chemical Physics, 2005, 7, 861. | 2.8 | 23 |
| 64 | Impact of Neighboring Chains on Torsional Defects in Oligothiophenes. Journal of Physical Chemistry A, 2012, 116, 2997-3003. | 2.5 | 23 |
| 65 | Endohedral and exohedral complexes of substituted benzenes with carbon nanotubes and graphene. Journal of Chemical Physics, 2013, 139, 094703. | 3.0 | 22 |
| 66 | Stacking Interactions between 9-Methyladenine and Heterocycles Commonly Found in Pharmaceuticals. Journal of Chemical Information and Modeling, 2016, 56, 906-914. | 5.4 | 22 |
| 67 | Ionization potentials of small lithium clusters (Lin) and hydrogenated lithium clusters (LinH). Journal of Chemical Physics, 2005, 122, 204328. | 3.0 | 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. | 5.4 | 21 |
| 69 | Remarkable electron accepting properties of the simplest benzenoid cyanocarbons: hexacyanobenzene, octacyanonaphthalene and decacyanoanthracene. Chemical Communications, 2006, , 758. | 4.1 | 20 |
| 70 | Harnessing weak interactions for enantioselective catalysis. Science, 2015, 347, 719-720. | 12.6 | 20 |
| 71 | Ring-Walking of Zerovalent Nickel on Aryl Halides. Journal of Chemical Theory and Computation, 2017, 13, 1706-1711. | 5.3 | 19 |
| 72 | SASS: A symmetry adapted stochastic search algorithm exploiting site symmetry. Journal of Chemical Physics, 2007, 126, 104104. | 3.0 | 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. | 2.8 | 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. | 13.8 | 17 |
| 75 | Conformational behavior and stacking interactions of contorted polycyclic aromatics. Physical Chemistry Chemical Physics, 2017, 19, 18186-18193. | 2.8 | 17 |
| 76 | 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 |
| 77 | 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 |
| 78 | The Pentacyanocyclopentadienyl System:Â Structures and Energetics. Journal of Physical Chemistry A, 2005, 109, 10084-10091. | 2.5 | 16 |
| 79 | Revised Role of Selectfluor in Homogeneous Auâ€Catalyzed Oxidative Cï£¿O Bond Formations. Chemistry - A European Journal, 2014, 20, 15833-15839. | 3.3 | 16 |
| 80 | On the convergence of Z-averaged perturbation theory. Journal of Chemical Physics, 2008, 128, 074107. | 3.0 | 15 |
| 81 | Stacked homodimers of substituted contorted hexabenzocoronenes and their complexes with C<sub>60</sub> fullerene. Organic and Biomolecular Chemistry, 2017, 15, 6042-6049. | 2.8 | 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. | 3.3 | 14 |
| 83 | Protonated carbonyl sulfide: Prospects for the spectroscopic observation of the elusive HSCO+ isomer. Journal of Chemical Physics, 2006, 124, 044322. | 3.0 | 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. | 2.5 | 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. | 2.6 | 12 |
| 86 | Stacking and Electrostatic Interactions Drive the Stereoselectivity of Silyliumâ€Ion Asymmetric Counteranionâ€Directed Catalysis. Angewandte Chemie, 2016, 128, 16121-16125. | 2.0 | 11 |
| 87 | Enantioselective Synthesis of Chiral Oxime Ethers: Desymmetrization and Dynamic Kinetic Resolution of Substituted Cyclohexanones. Angewandte Chemie, 2017, 129, 2494-2498. | 2.0 | 11 |
| 88 | Reactive ligand influence on initiation in phenylene catalystâ€transfer polymerization. Journal of Polymer Science Part A, 2017, 55, 1530-1535. | 2.3 | 11 |
| 89 | Converting SMILES to Stacking Interaction Energies. Journal of Chemical Information and Modeling, 2019, 59, 3413-3421. | 5.4 | 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. | 3.3 | 11 |

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| 91 | Hydrogen-Abstracted Adenineâ^'Thymine Radicals with Interesting Transferable Properties. Journal of Physical Chemistry B, 2007, 111, 5525-5530. | 2.6 | 10 |
| 92 | Vibrational Spectroscopy and Theory of the Protonated Benzene Dimer and Trimer. Journal of Physical Chemistry A, 2012, 116, 7065-7073. | 2.5 | 10 |
| 93 | Optimization of Catalyst Structure for Asymmetric Propargylation of Aldehydes with Allenyltrichlorosilane. Advanced Synthesis and Catalysis, 2020, 362, 5467-5474. | 4.3 | 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. | 3.1 | 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. | 3.2 | 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. | 2.6 | 7 |
| 97 | The extremely flat torsional potential energy surface of oxalyl chloride. Journal of Chemical Physics, 2005, 122, 234313. | 3.0 | 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. | 2.5 | 6 |
| 99 | Rennerâ^'Teller Bending Frequencies of the Ãƒ 2Î State of OCS+. Journal of Physical Chemistry A, 2007, 111, 4551-4555. | 2.5 | 5 |
| 100 | Automated Quantum Mechanical Predictions of Enantioselectivity in a Rhodiumâ€Catalyzed Asymmetric Hydrogenation. Angewandte Chemie, 2017, 129, 9229-9233. | 2.0 | 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. | 4.5 | 5 |
| 102 | Importance of favourable non-covalent contacts in the stereoselective synthesis of tetrasubstituted chromanones. Organic Chemistry Frontiers, 2022, 9, 3027-3033. | 4.5 | 5 |
| 103 | Importance of model size in quantum mechanical studies of DNA intercalation. Journal of Computational Chemistry, 2020, 41, 1175-1184. | 3.3 | 4 |
| 104 | Mechanism and Origin of Selectivity in Platinum(II)â€Catalyzed Reactions of Acyclic Î³,Î´â€¥nones with Alkenes. ChemCatChem, 2016, 8, 2771-2780. | 3.7 | 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. | 3.2 | 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. | 2.0 | 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, , . | 5.5 | 1 |