Kendall N Houk

List of Publications by Year
in descending order

108 papers	13,859 citations	46918 47 h-index	24179 110 g-index
124 all docs	124 docs citations	124 times ranked	11639 citing authors

#	Article	IF	Citations
1	Kemp elimination catalysts by computational enzyme design. Nature, 2008, 453, 190-195.	13.7	1,130
2	Analyzing Reaction Rates with the Distortion/Interactionâ€Activation Strain Model. Angewandte Chemie - International Edition, 2017, 56, 10070-10086.	7.2	1,060
3	De Novo Computational Design of Retro-Aldol Enzymes. Science, 2008, 319, 1387-1391.	6.0	1,031
4	Constructive molecular configurations for surface-defect passivation of perovskite photovoltaics. Science, 2019, 366, 1509-1513.	6.0	846
5	Computational Design of an Enzyme Catalyst for a Stereoselective Bimolecular Diels-Alder Reaction. Science, 2010, 329, 309-313.	6.0	776
6	Frontier molecular orbital theory of cycloaddition reactions. Accounts of Chemical Research, 1975, 8, 361-369.	7.6	733
7	Pericyclic Reaction Transition States: Passions and Punctilios, 1935-1995. Accounts of Chemical Research, 1995, 28, 81-90.	7.6	626
8	Transition Structures of Hydrocarbon Pericyclic Reactions. Angewandte Chemie International Edition in English, 1992, 31, 682-708.	4.4	586
9	A Hierarchy of Homodesmotic Reactions for Thermochemistry. Journal of the American Chemical Society, 2009, 131, 2547-2560.	6.6	508
10	The reduction potential of nitric oxide (NO) and its importance to NO biochemistry. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 10958-10963.	3.3	339
11	Bifurcations on Potential Energy Surfaces of Organic Reactions. Angewandte Chemie - International Edition, 2008, 47, 7592-7601.	7.2	316
12	Iterative approach to computational enzyme design. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 3790-3795.	3.3	291
13	Theozymes and compuzymes: theoretical models for biological catalysis. Current Opinion in Chemical Biology, 1998, 2, 743-750.	2.8	223
14	Palladium-Catalyzed Suzukiâ€"Miyaura Coupling of Aryl Esters. Journal of the American Chemical Society, 2017, 139, 1311-1318.	6.6	212
15	Das Distortion/Interactionâ€Activationâ€Strainâ€Modell zur Analyse von Reaktionsgeschwindigkeiten. Angewandte Chemie, 2017, 129, 10204-10221.	1.6	209
16	Bridging the gaps in design methodologies by evolutionary optimization of the stability and proficiency of designed Kemp eliminase KE59. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 10358-10363.	3.3	205
17	The Concept of Protobranching and Its Many Paradigm Shifting Implications for Energy Evaluations. Chemistry - A European Journal, 2007, 13, 7731-7744.	1.7	185
18	Metal-free directed sp2-Câ€"H borylation. Nature, 2019, 575, 336-340.	13.7	175

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19	From Porphyrin Isomers to Octapyrrolicâ€œFigure Eightâ€•Macrocycles. Angewandte Chemie International Edition in English, 1995, 34, 2511-2514.	4.4	168
20	Dynamics, transition states, and timing of bond formation in Dielsâ€“Alder reactions. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 12860-12865.	3.3	166
21	Sources of Error in DFT Computations of Cï£¿C Bond Formation Thermochemistries: Ï€â†'Ïƒ Transformations and Error Cancellation by DFT Methods. Angewandte Chemie - International Edition, 2008, 47, 7746-7749.	7.2	162
22	Nickelâ€Catalyzed Activation of Acyl Câˆ'O Bonds of Methyl Esters. Angewandte Chemie - International Edition, 2016, 55, 2810-2814.	7.2	142
23	An Antibody exo Diels-Alderase Inhibitor Complex at 1.95 Angstrom Resolution. Science, 1998, 279, 1934-1940.	6.0	141
24	A promiscuous cytochrome P450 aromatic O-demethylase for lignin bioconversion. Nature Communications, 2018, 9, 2487.	5.8	135
25	BrÃ¸nsted Acid Catalyzed Asymmetric Propargylation of Aldehydes. Angewandte Chemie - International Edition, 2012, 51, 1391-1394.	7.2	124
26	Photochemical intermolecular dearomative cycloaddition of bicyclic azaarenes with alkenes. Science, 2021, 371, 1338-1345.	6.0	119
27	Enzymatic catalysis of anti-Baldwin ring closure in polyether biosynthesis. Nature, 2012, 483, 355-358.	13.7	117
28	Evolution of Shape Complementarity and Catalytic Efficiency from a Primordial Antibody Template. Science, 1999, 286, 2345-2348.	6.0	116
29	Ãœbergangsstrukturen in pericyclischen Reaktionen von Kohlenwasserstoffen. Angewandte Chemie, 1992, 104, 711-739.	1.6	111
30	Origins of stereoselectivity in evolved ketoreductases. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E7065-72.	3.3	104
31	The Origin of the Halogen Effect on Reactivity and Reversibility of Dielsâ€“Alder Cycloadditions Involving Furan. Angewandte Chemie - International Edition, 2006, 45, 1442-1445.	7.2	97
32	The Chemistry and Biology of Nitroxyl (HNO): A Chemically Unique Species with Novel and Important Biological Activity. ChemBioChem, 2005, 6, 612-619.	1.3	95
33	Cycloaddition Reactions of Butadiene and 1,3â€Dipoles to Curved Arenes, Fullerenes, and Nanotubes: Theoretical Evaluation of the Role of Distortion Energies on Activation Barriers. Chemistry - A European Journal, 2009, 15, 13219-13231.	1.7	92
34	High-Yield Sorting of Small-Diameter Carbon Nanotubes for Solar Cells and Transistors. ACS Nano, 2014, 8, 2609-2617.	7.3	91
35	Scalable and Selective Dispersion of Semiconducting Arc-Discharged Carbon Nanotubes by Dithiafulvalene/Thiophene Copolymers for Thin Film Transistors. ACS Nano, 2013, 7, 2659-2668.	7.3	88
36	Evolution of the Dielsâ€“Alder Reaction Mechanism since the 1930s: Woodward, Houk with Woodward, and the Influence of Computational Chemistry on Understanding Cycloadditions. Angewandte Chemie - International Edition, 2021, 60, 12660-12681.	7.2	85

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37	Transition structures for the allylboration reactions of formaldehyde by allylborane and allylboronic acid. Journal of the American Chemical Society, 1989, 111, 1236-1240.	6.6	83
38	Enzyme-catalysed [6+4] cycloadditions in the biosynthesis of natural products. Nature, 2019, 568, 122-126.	13.7	83
39	Theoretical Reduction Potentials for Nitrogen Oxides from CBS-QB3 Energetics and (C)PCM Solvation Calculations. Inorganic Chemistry, 2005, 44, 4024-4028.	1.9	82
40	Involvement of Lipocalinâ€like CghA in Decalinâ€Forming Stereoselective Intramolecular [4+2] Cycloaddition. ChemBioChem, 2015, 16, 2294-2298.	1.3	80
41	Structural Basis for Antibody Catalysis of a Disfavored Ring Closure Reaction,. Biochemistry, 1999, 38, 7062-7074.	1.2	69
42	Solvent Effects on Polymer Sorting of Carbon Nanotubes with Applications in Printed Electronics. Small, 2015, 11, 126-133.	5.2	69
43	Thermodynamics of the Conversion of Chorismate to Prephenate:â€‰ Experimental Results and Theoretical Predictions. Journal of Physical Chemistry B, 1997, 101, 10976-10982.	1.2	58
44	Influence of water and enzyme SpnF on the dynamics and energetics of the ambimodal [6+4]/[4+2] cycloaddition. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E848-E855.	3.3	57
45	Performance-limiting formation dynamics in mixed-halide perovskites. Science Advances, 2021, 7, eabj1799.	4.7	54
46	Mild Ringâ€Opening 1,3â€Hydroborations of Nonâ€Activated Cyclopropanes. Angewandte Chemie - International Edition, 2018, 57, 16861-16865.	7.2	52
47	Unexpected regioselectivity in the reductive cleavage of epoxides: a theoretical rationalization. Journal of the American Chemical Society, 1989, 111, 8976-8978.	6.6	51
48	Engineering synthetic recursive pathways to generate non-natural small molecules. Nature Chemical Biology, 2012, 8, 518-526.	3.9	51
49	Structural Distortion of Cycloalkynes Influences Cycloaddition Rates both by Strain and Interaction Energies. Chemistry - A European Journal, 2019, 25, 6342-6348.	1.7	49
50	Nitrone Ionization Potentials and Cycloaddition Regioselectivities. Heterocycles, 1977, 7, 293.	0.4	48
51	Fluorineâ€Directed Diastereoselective Iodocyclizations. Angewandte Chemie - International Edition, 2008, 47, 357-360.	7.2	45
52	Pericyclic Cascade with Chirality Transfer: Reaction Pathway and Origin of Enantioselectivity of the Heteroâ€Claisen Approach to Oxindoles. Angewandte Chemie - International Edition, 2011, 50, 11478-11482.	7.2	45
53	Polyether Catalysis of Ester Aminolysis â€" A Computational and Experimental Study. Liebigs Annalen, 1996, 1996, 1511-1522.	0.8	44
54	Theoretical and experimental insights into cycloaddition reactions. , 1979, , 1-40.		42

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55	Chiral Phosphoric Acid Dualâ€Function Catalysis: Asymmetric Allylation with Î±â€Vinyl Allylboron Reagents. Angewandte Chemie - International Edition, 2020, 59, 10540-10548.	7.2	42
56	Facile access to fused 2D/3D rings via intermolecular cascade dearomative [2â€‰+â€‰2] cycloaddition/rearrangement reactions of quinolines with alkenes. Nature Catalysis, 2022, 5, 405-413.	16.1	42
57	Enabling microbial syringol conversion through structure-guided protein engineering. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 13970-13976.	3.3	41
58	Synthetic, Mechanistic, and Biological Interrogation of <i>Ginkgo biloba</i> Chemical Space En Route to (âˆ’)-Bilobalide. Journal of the American Chemical Society, 2020, 142, 18599-18618.	6.6	40
59	Metalâ€Free Directed Câˆ’H Borylation of Pyrroles. Angewandte Chemie - International Edition, 2021, 60, 8500-8504.	7.2	40
60	Synthesis of [¹⁸F]Fluoroarenes by Nucleophilic Radiofluorination of <i>N</i>â€Arylsydnones. Angewandte Chemie - International Edition, 2017, 56, 13006-13010.	7.2	39
61	A Convergent Strategy for the Asymmetric Synthesis of Enantiomerically Pure Bicyclic Compounds by Using a Silicon-Directed Cycloaddition Reaction: The Synthesis of Enantiomerically Pure Bicyclo[3.2.0]hept-2-en-6-one. Angewandte Chemie - International Edition, 1999, 38, 2728-2730.	7.2	36
62	Catalytic mechanism and endo-to-exo selectivity reversion of an octalin-forming natural Dielsâ€“Alderase. Nature Catalysis, 2021, 4, 223-232.	16.1	35
63	Structures and Stabilities of Diacetylene-Expanded Polyhedranes by Quantum Mechanics and Molecular Mechanics. Journal of Organic Chemistry, 2005, 70, 1671-1678.	1.7	33
64	Axial Preferences in Allylations via the Zimmermanâ€“Traxler Transition State. Chemistry - A European Journal, 2011, 17, 8000-8004.	1.7	33
65	Mild Ringâ€Opening 1,3â€Hydroborations of Nonâ€Activated Cyclopropanes. Angewandte Chemie, 2018, 130, 17103-17107.	1.6	33
66	Nâ€Type Conjugated Polymerâ€Enabled Selective Dispersion of Semiconducting Carbon Nanotubes for Flexible CMOSâ€Like Circuits. Advanced Functional Materials, 2015, 25, 1837-1844.	7.8	32
67	The Influence of Constitutional Isomerism and Change on Molecular Recognition Processes. Chemistry - A European Journal, 2004, 10, 5406-5421.	1.7	28
68	Competition Between Concerted and Stepwise Dynamics in the Triplet Diâ€Ï€â€Methane Rearrangement. Angewandte Chemie - International Edition, 2014, 53, 8664-8667.	7.2	28
69	autoDIAS: a python tool for an automated distortion/interaction activation strain analysis. Journal of Computational Chemistry, 2019, 40, 2509-2515.	1.5	28
70	Stereochemical Control via Chirality Pairing: Stereodivergent Syntheses of Enantioenriched Homoallylic Alcohols. Angewandte Chemie - International Edition, 2021, 60, 24096-24106.	7.2	28
71	Investigation of Trimethyllysine Binding by the HP1 Chromodomain via Unnatural Amino Acid Mutagenesis. Journal of the American Chemical Society, 2017, 139, 17253-17256.	6.6	27
72	Forming Tertiary Organolithiums and Organocuprates from Nitrile Precursors and their Bimolecular Reactions with Carbon Electrophiles to Form Quaternary Carbon Stereocenters. Angewandte Chemie - International Edition, 2012, 51, 9581-9586.	7.2	26

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73	Enantioselective Homocrotylboration of Aliphatic Aldehydes. Journal of the American Chemical Society, 2013, 135, 82-85.	6.6	26
74	Origins of <i>Endo</i> Selectivity in Dielsâ€“Alder Reactions of Cyclic Allene Dienophiles. Angewandte Chemie - International Edition, 2021, 60, 14989-14997.	7.2	24
75	Direct Synthesis of Ketones from Methyl Esters by Nickelâ€Catalyzed Suzukiâ€“Miyaura Coupling. Angewandte Chemie - International Edition, 2021, 60, 13476-13483.	7.2	22
76	Reactivity of Singleâ€Walled Carbon Nanotubes in the Dielsâ€“Alder Cycloaddition Reaction: Distortionâ€“Interaction Analysis along the Reaction Pathway. Chemistry - A European Journal, 2016, 22, 12819-12824.	1.7	21
77	Thermodynamic and Quantum Chemical Study of the Conversion of Chorismate to (Pyruvate +) Tj ETQq1 1 0.784314 rgBT /Overlock 10	1.2	19
78	Chiral Phosphoric Acid Catalyzed Conversion of Epoxides into Thiiranes: Mechanism, Stereochemical Model, and New Catalyst Design. Angewandte Chemie - International Edition, 2022, 61, .	7.2	19
79	Aromatic Claisen Rearrangements of <i>O</i>â€Prenylated Tyrosine and Model Prenyl Aryl Ethers: Computational Study of the Role of Water on Acceleration of Claisen Rearrangements. European Journal of Organic Chemistry, 2013, 2013, 2823-2831.	1.2	18
80	How the Lewis Base F^{â€“}Catalyzes the 1,3-Dipolar Cycloaddition between Carbon Dioxide and Nitrilimines. Journal of Organic Chemistry, 2021, 86, 4320-4325.	1.7	17
81	Palladiumkomplexe der neuen Porphyrinisomere (<i>Z</i>)â€•und (<i>E</i>)â€Isoporphycen â€“ Pd^{<scp>II</scp>}â€induzierte Cyclisierungen von Tetrapyrrolaldehyden. Angewandte Chemie, 1997, 109, 363-367.	1.6	16
82	Transition Structures of the Electrocyclic Reactions of <i>cis,cis,cis</i>â€1,3,5â€Cyclooctatriene. Israel Journal of Chemistry, 1993, 33, 287-293.	1.0	15
83	Understand the Specific Regio- and Enantioselectivity of Fluostatin Conjugation in the Post-Biosynthesis. Biomolecules, 2020, 10, 815.	1.8	15
84	Die Evolution des Dielsâ€Alderâ€Reaktionsmechanismus seit den 1930er Jahren: Woodward, Houk zusammen mit Woodward und der Einfluss der Computerchemie auf das VerstÃndnis von Cycloadditionen. Angewandte Chemie, 2021, 133, 12768-12790.	1.6	15
85	Cycloaddition Cascades of Strained Alkynes and Oxadiazinones. Angewandte Chemie - International Edition, 2021, 60, 18201-18208.	7.2	15
86	Computationally designed ligands enable tunable borylation of remote Câ€“H bonds in arenes. CheM, 2022, 8, 1775-1788.	5.8	14
87	Fluorine as a Regiocontrol Element in the Ring Opening of Bicyclic Aziridiniums. Helvetica Chimica Acta, 2012, 95, 2265-2277.	1.0	13
88	Rolf Huisgen's Classic Studies of Cyclic Triene Dielsâ€“Alder Reactions Elaborated by Modern Computational Analysis. Angewandte Chemie - International Edition, 2020, 59, 12506-12519.	7.2	13
89	Systematic Variation of Both the Aromatic Cage and Dialkyllysine via GCE-SAR Reveal Mechanistic Insights in CBX5 Reader Protein Binding. Journal of Medicinal Chemistry, 2022, 65, 2646-2655.	2.9	13
90	Computational Protocol to Understand P450 Mechanisms and Design of Efficient and Selective Biocatalysts. Frontiers in Chemistry, 2018, 6, 663.	1.8	12

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91	Metalâ€Free Directed Câˆ’H Borylation of Pyrroles. Angewandte Chemie, 2021, 133, 8581-8585.	1.6	12
92	Computational Exploration of Ambiphilic Reactivity of Azides and Sustmannâ€™s Paradigmatic Parabola. Journal of Organic Chemistry, 2021, 86, 5792-5804.	1.7	11
93	Synthesis of [¹⁸F]Fluoroarenes by Nucleophilic Radiofluorination of <i>N</i>â€Arylsydnones. Angewandte Chemie, 2017, 129, 13186-13190.	1.6	10
94	Chiral Phosphoric Acid Dualâ€Function Catalysis: Asymmetric Allylation with Î±â€Vinyl Allylboron Reagents. Angewandte Chemie, 2020, 132, 10627-10635.	1.6	10
95	Stereochemical Control via Chirality Pairing: Stereodivergent Syntheses of Enantioenriched Homoallylic Alcohols. Angewandte Chemie, 2021, 133, 24298-24308.	1.6	8
96	Stereodivergent Attachedâ€Ring Synthesis via Nonâ€Covalent Interactions: A Short Formal Synthesis of Merrilactone A. Angewandte Chemie - International Edition, 2022, 61, .	7.2	8
97	Theoretical enzyme design using the Kepler scientific workflows on the Grid. Procedia Computer Science, 2010, 1, 1175-1184.	1.2	7
98	Understanding the R882H mutation effects of DNA methyltransferase DNMT3A: a combination of molecular dynamics simulations and QM/MM calculations. RSC Advances, 2019, 9, 31425-31434.	1.7	7
99	Direct Synthesis of Ketones from Methyl Esters by Nickelâ€Catalyzed Suzukiâ€"Miyaura Coupling. Angewandte Chemie, 2021, 133, 13588-13595.	1.6	7
100	Chiral Phosphoric Acid Catalyzed Conversion of Epoxides into Thiiranes: Mechanism, Stereochemical Model, and New Catalyst Design. Angewandte Chemie, 0, , .	1.6	6
101	Facilitating e-Science Discovery Using Scientific Workflows on the Grid. Computer Communications and Networks, 2011, , 353-382.	0.8	5
102	Cycloaddition Cascades of Strained Alkynes and Oxadiazinones. Angewandte Chemie, 2021, 133, 18349-18356.	1.6	4
103	Origins of Endo Selectivity in Dielsâ€"Alder Reactions of Cyclic Allene Dienophiles. Angewandte Chemie, 2021, 133, 15116-15124.	1.6	3
104	Control of Hetero-Diels-Alder Stereoselectivity through Solvent Polarity and BrÃ¸nsted or Lewis Acid Catalysis; Theory and Experiment. Synlett, 2013, 24, 2446-2450.	1.0	2
105	Organic Chemistry and Synthesis Rely More and More upon Catalysts. Catalysts, 2022, 12, 758.	1.6	2
106	Rolf Huisgen's Classic Studies of Cyclic Triene Dielsâ€"Alder Reactions Elaborated by Modern Computational Analysis. Angewandte Chemie, 2020, 132, 12606-12619.	1.6	1
107	John D. Roberts, his beginnings at UCLA, his transformation of physical organic chemistry, and his impact on science. Journal of Physical Organic Chemistry, 2018, 31, e3810.	0.9	0
108	Stereodivergent Attachedâ€Ring Synthesis via Nonâ€Covalent Interactions: A Short Formal Synthesis of Merrilactone A. Angewandte Chemie, 2022, 134, e202114514.	1.6	0