

Kendall N Houk

List of Publications by Year in descending order

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108
papers

13,859
citations

47006

47
h-index

24258

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. <i>Nature</i> , 2008, 453, 190-195.	27.8	1,130
2	Analyzing Reaction Rates with the Distortion/Interaction-Activation Strain Model. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 10070-10086.	13.8	1,060
3	De Novo Computational Design of Retro-Aldol Enzymes. <i>Science</i> , 2008, 319, 1387-1391.	12.6	1,031
4	Constructive molecular configurations for surface-defect passivation of perovskite photovoltaics. <i>Science</i> , 2019, 366, 1509-1513.	12.6	846
5	Computational Design of an Enzyme Catalyst for a Stereoselective Bimolecular Diels-Alder Reaction. <i>Science</i> , 2010, 329, 309-313.	12.6	776
6	Frontier molecular orbital theory of cycloaddition reactions. <i>Accounts of Chemical Research</i> , 1975, 8, 361-369.	15.6	733
7	Pericyclic Reaction Transition States: Passions and Punctilios, 1935-1995. <i>Accounts of Chemical Research</i> , 1995, 28, 81-90.	15.6	626
8	Transition Structures of Hydrocarbon Pericyclic Reactions. <i>Angewandte Chemie International Edition in English</i> , 1992, 31, 682-708.	4.4	586
9	A Hierarchy of Homodesmotic Reactions for Thermochemistry. <i>Journal of the American Chemical Society</i> , 2009, 131, 2547-2560.	13.7	508
10	The reduction potential of nitric oxide (NO) and its importance to NO biochemistry. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002, 99, 10958-10963.	7.1	339
11	Bifurcations on Potential Energy Surfaces of Organic Reactions. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 7592-7601.	13.8	316
12	Iterative approach to computational enzyme design. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 3790-3795.	7.1	291
13	Theozymes and compuzymes: theoretical models for biological catalysis. <i>Current Opinion in Chemical Biology</i> , 1998, 2, 743-750.	6.1	223
14	Palladium-Catalyzed Suzuki-Miyaura Coupling of Aryl Esters. <i>Journal of the American Chemical Society</i> , 2017, 139, 1311-1318.	13.7	212
15	Das Distortion/Interaction-Activation-Strain-Modell zur Analyse von Reaktionsgeschwindigkeiten. <i>Angewandte Chemie</i> , 2017, 129, 10204-10221.	2.0	209
16	Bridging the gaps in design methodologies by evolutionary optimization of the stability and proficiency of designed Kemp eliminase KE59. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 10358-10363.	7.1	205
17	The Concept of Protobranching and Its Many Paradigm Shifting Implications for Energy Evaluations. <i>Chemistry - A European Journal</i> , 2007, 13, 7731-7744.	3.3	185
18	Metal-free directed sp ² -C-H borylation. <i>Nature</i> , 2019, 575, 336-340.	27.8	175

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19	From Porphyrin Isomers to Octapyrrolic "Figure Eight" Macrocycles. <i>Angewandte Chemie International Edition in English</i> , 1995, 34, 2511-2514.	4.4	168
20	Dynamics, transition states, and timing of bond formation in Diels-Alder reactions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 12860-12865.	7.1	166
21	Sources of Error in DFT Computations of C-C Bond Formation Thermochemistries: Identification Transformations and Error Cancellation by DFT Methods. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 7746-7749.	13.8	162
22	Nickel-Catalyzed Activation of Acyl C=O Bonds of Methyl Esters. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 2810-2814.	13.8	142
23	An Antibody exo Diels-Alderase Inhibitor Complex at 1.95 Å Resolution. <i>Science</i> , 1998, 279, 1934-1940.	12.6	141
24	A promiscuous cytochrome P450 aromatic O-demethylase for lignin bioconversion. <i>Nature Communications</i> , 2018, 9, 2487.	12.8	135
25	Brønsted Acid Catalyzed Asymmetric Propargylation of Aldehydes. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 1391-1394.	13.8	124
26	Photochemical intermolecular dearomative cycloaddition of bicyclic azaarenes with alkenes. <i>Science</i> , 2021, 371, 1338-1345.	12.6	119
27	Enzymatic catalysis of anti-Baldwin ring closure in polyether biosynthesis. <i>Nature</i> , 2012, 483, 355-358.	27.8	117
28	Evolution of Shape Complementarity and Catalytic Efficiency from a Primordial Antibody Template. <i>Science</i> , 1999, 286, 2345-2348.	12.6	116
29	Übergangsstrukturen in pericyclischen Reaktionen von Kohlenwasserstoffen. <i>Angewandte Chemie</i> , 1992, 104, 711-739.	2.0	111
30	Origins of stereoselectivity in evolved ketoreductases. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, E7065-72.	7.1	104
31	The Origin of the Halogen Effect on Reactivity and Reversibility of Diels-Alder Cycloadditions Involving Furan. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 1442-1445.	13.8	97
32	The Chemistry and Biology of Nitroxyl (HNO): A Chemically Unique Species with Novel and Important Biological Activity. <i>ChemBioChem</i> , 2005, 6, 612-619.	2.6	95
33	Cycloaddition Reactions of Butadiene and 1,3-Dipoles to Curved Arenes, Fullerenes, and Nanotubes: Theoretical Evaluation of the Role of Distortion Energies on Activation Barriers. <i>Chemistry - A European Journal</i> , 2009, 15, 13219-13231.	3.3	92
34	High-Yield Sorting of Small-Diameter Carbon Nanotubes for Solar Cells and Transistors. <i>ACS Nano</i> , 2014, 8, 2609-2617.	14.6	91
35	Scalable and Selective Dispersion of Semiconducting Arc-Discharged Carbon Nanotubes by Dithiafulvalene/Thiophene Copolymers for Thin Film Transistors. <i>ACS Nano</i> , 2013, 7, 2659-2668.	14.6	88
36	Evolution of the Diels-Alder Reaction Mechanism since the 1930s: Woodward, Houk with Woodward, and the Influence of Computational Chemistry on Understanding Cycloadditions. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 12660-12681.	13.8	85

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37	Transition structures for the allylboration reactions of formaldehyde by allylborane and allylboronic acid. <i>Journal of the American Chemical Society</i> , 1989, 111, 1236-1240.	13.7	83
38	Enzyme-catalysed [6+4] cycloadditions in the biosynthesis of natural products. <i>Nature</i> , 2019, 568, 122-126.	27.8	83
39	Theoretical Reduction Potentials for Nitrogen Oxides from CBS-QB3 Energetics and (C)PCM Solvation Calculations. <i>Inorganic Chemistry</i> , 2005, 44, 4024-4028.	4.0	82
40	Involvement of Lipocalin-like CghA in Decalin-Forming Stereoselective Intramolecular [4+2] Cycloaddition. <i>ChemBioChem</i> , 2015, 16, 2294-2298.	2.6	80
41	Structural Basis for Antibody Catalysis of a Disfavored Ring Closure Reaction,. <i>Biochemistry</i> , 1999, 38, 7062-7074.	2.5	69
42	Solvent Effects on Polymer Sorting of Carbon Nanotubes with Applications in Printed Electronics. <i>Small</i> , 2015, 11, 126-133.	10.0	69
43	Thermodynamics of the Conversion of Chorismate to Prephenate: Experimental Results and Theoretical Predictions. <i>Journal of Physical Chemistry B</i> , 1997, 101, 10976-10982.	2.6	58
44	Influence of water and enzyme SpnF on the dynamics and energetics of the ambimodal [6+4]/[4+2] cycloaddition. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E848-E855.	7.1	57
45	Performance-limiting formation dynamics in mixed-halide perovskites. <i>Science Advances</i> , 2021, 7, eabj1799.	10.3	54
46	Mild Ring-Opening 1,3-Hydroborations of Non-Activated Cyclopropanes. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 16861-16865.	13.8	52
47	Unexpected regioselectivity in the reductive cleavage of epoxides: a theoretical rationalization. <i>Journal of the American Chemical Society</i> , 1989, 111, 8976-8978.	13.7	51
48	Engineering synthetic recursive pathways to generate non-natural small molecules. <i>Nature Chemical Biology</i> , 2012, 8, 518-526.	8.0	51
49	Structural Distortion of Cycloalkynes Influences Cycloaddition Rates both by Strain and Interaction Energies. <i>Chemistry - A European Journal</i> , 2019, 25, 6342-6348.	3.3	49
50	Nitrene Ionization Potentials and Cycloaddition Regioselectivities. <i>Heterocycles</i> , 1977, 7, 293.	0.7	48
51	Fluorine-Directed Diastereoselective Iodocyclizations. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 357-360.	13.8	45
52	Pericyclic Cascade with Chirality Transfer: Reaction Pathway and Origin of Enantioselectivity of the Hetero-Claisen Approach to Oxindoles. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 11478-11482.	13.8	45
53	Polyether Catalysis of Ester Aminolysis – A Computational and Experimental Study. <i>Liebigs Annalen</i> , 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 Dual-Function Catalysis: Asymmetric Allylation with \pm -Vinyl Allylboron Reagents. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 10540-10548.	13.8	42
56	Facile access to fused 2D/3D rings via intermolecular cascade dearomative [2+2] cycloaddition/rearrangement reactions of quinolines with alkenes. <i>Nature Catalysis</i> , 2022, 5, 405-413.	34.4	42
57	Enabling microbial syringol conversion through structure-guided protein engineering. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 13970-13976.	7.1	41
58	Synthetic, Mechanistic, and Biological Interrogation of <i>Ginkgo biloba</i> Chemical Space En Route to ($\hat{\alpha}$)-Bilobalide. <i>Journal of the American Chemical Society</i> , 2020, 142, 18599-18618.	13.7	40
59	Metal-Free Directed C-H Borylation of Pyrroles. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 8500-8504.	13.8	40
60	Synthesis of [¹⁸ F]Fluoroarenes by Nucleophilic Radiofluorination of Arylsydnone. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 13006-13010.	13.8	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. <i>Angewandte Chemie - International Edition</i> , 1999, 38, 2728-2730.	13.8	36
62	Catalytic mechanism and endo-to-exo selectivity reversion of an octalin-forming natural Diels-Alderase. <i>Nature Catalysis</i> , 2021, 4, 223-232.	34.4	35
63	Structures and Stabilities of Diacetylene-Expanded Polyhedranes by Quantum Mechanics and Molecular Mechanics. <i>Journal of Organic Chemistry</i> , 2005, 70, 1671-1678.	3.2	33
64	Axial Preferences in Allylations via the Zimmerman-Traxler Transition State. <i>Chemistry - A European Journal</i> , 2011, 17, 8000-8004.	3.3	33
65	Mild Ring-Opening 1,3-Hydroborations of Non-Activated Cyclopropanes. <i>Angewandte Chemie</i> , 2018, 130, 17103-17107.	2.0	33
66	N-Type Conjugated Polymer-Enabled Selective Dispersion of Semiconducting Carbon Nanotubes for Flexible CMOS-Like Circuits. <i>Advanced Functional Materials</i> , 2015, 25, 1837-1844.	14.9	32
67	The Influence of Constitutional Isomerism and Change on Molecular Recognition Processes. <i>Chemistry - A European Journal</i> , 2004, 10, 5406-5421.	3.3	28
68	Competition Between Concerted and Stepwise Dynamics in the Triplet Diene-Methane Rearrangement. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 8664-8667.	13.8	28
69	autoDIAS: a python tool for an automated distortion/interaction activation strain analysis. <i>Journal of Computational Chemistry</i> , 2019, 40, 2509-2515.	3.3	28
70	Stereochemical Control via Chirality Pairing: Stereodivergent Syntheses of Enantioenriched Homoallylic Alcohols. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 24096-24106.	13.8	28
71	Investigation of Trimethyllysine Binding by the HP1 Chromodomain via Unnatural Amino Acid Mutagenesis. <i>Journal of the American Chemical Society</i> , 2017, 139, 17253-17256.	13.7	27
72	Forming Tertiary Organolithiums and Organocuprates from Nitrile Precursors and their Bimolecular Reactions with Carbon Electrophiles to Form Quaternary Carbon Stereocenters. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 9581-9586.	13.8	26

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73	Enantioselective Homocrotlylboration of Aliphatic Aldehydes. <i>Journal of the American Chemical Society</i> , 2013, 135, 82-85.	13.7	26
74	Origins of <i>Endo</i> Selectivity in Diels-Alder Reactions of Cyclic Allene Dienophiles. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 14989-14997.	13.8	24
75	Direct Synthesis of Ketones from Methyl Esters by Nickel-Catalyzed Suzuki-Miyaura Coupling. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 13476-13483.	13.8	22
76	Reactivity of Single-Walled Carbon Nanotubes in the Diels-Alder Cycloaddition Reaction: Distortion-Interaction Analysis along the Reaction Pathway. <i>Chemistry - A European Journal</i> , 2016, 22, 12819-12824.	3.3	21
77	Thermodynamic and Quantum Chemical Study of the Conversion of Chorismate to (Pyruvate +) Tj ETQq1 1 0.784314 rgBT /Overlock 10	2.6	19
78	Chiral Phosphoric Acid Catalyzed Conversion of Epoxides into Thiiranes: Mechanism, Stereochemical Model, and New Catalyst Design. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	19
79	Aromatic Claisen Rearrangements of <i>O</i> -Prenylated Tyrosine and Model Prenyl Aryl Ethers: Computational Study of the Role of Water on Acceleration of Claisen Rearrangements. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 2823-2831.	2.4	18
80	How the Lewis Base F^{-} Catalyzes the 1,3-Dipolar Cycloaddition between Carbon Dioxide and Nitrilimines. <i>Journal of Organic Chemistry</i> , 2021, 86, 4320-4325.	3.2	17
81	Palladiumkomplexe der neuen Porphyrinisomere (<i>Z</i>)- und (<i>E</i>)-isoporphycen -induzierte Cyclisierungen von Tetrapyrrolaldehyden. <i>Angewandte Chemie</i> , 1997, 109, 363-367.	2.0	16
82	Transition Structures of the Electrocyclic Reactions of <i>cis,cis,cis</i> -1,3,5-Cyclooctatriene. <i>Israel Journal of Chemistry</i> , 1993, 33, 287-293.	2.3	15
83	Understand the Specific Regio- and Enantioselectivity of Fluostatin Conjugation in the Post-Biosynthesis. <i>Biomolecules</i> , 2020, 10, 815.	4.0	15
84	Die Evolution des Diels-Alder-Reaktionsmechanismus seit den 1930er Jahren: Woodward, Houk zusammen mit Woodward und der Einfluss der Computerchemie auf das VerstÄndnis von Cycloadditionen. <i>Angewandte Chemie</i> , 2021, 133, 12768-12790.	2.0	15
85	Cycloaddition Cascades of Strained Alkynes and Oxadiazinones. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 18201-18208.	13.8	15
86	Computationally designed ligands enable tunable borylation of remote C-H bonds in arenes. <i>Chem</i> , 2022, 8, 1775-1788.	11.7	14
87	Fluorine as a Regiocontrol Element in the Ring Opening of Bicyclic Aziridiniums. <i>Helvetica Chimica Acta</i> , 2012, 95, 2265-2277.	1.6	13
88	Rolf Huisgen's Classic Studies of Cyclic Triene Diels-Alder Reactions Elaborated by Modern Computational Analysis. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 12506-12519.	13.8	13
89	Systematic Variation of Both the Aromatic Cage and Dialkyllysine via GCE-SAR Reveal Mechanistic Insights in CBX5 Reader Protein Binding. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 2646-2655.	6.4	13
90	Computational Protocol to Understand P450 Mechanisms and Design of Efficient and Selective Biocatalysts. <i>Frontiers in Chemistry</i> , 2018, 6, 663.	3.6	12

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91	Metal-Free Directed C-H Borylation of Pyrroles. <i>Angewandte Chemie</i> , 2021, 133, 8581-8585.	2.0	12
92	Computational Exploration of Ambiphilic Reactivity of Azides and Sustmann's Paradigmatic Parabola. <i>Journal of Organic Chemistry</i> , 2021, 86, 5792-5804.	3.2	11
93	Synthesis of [¹⁸ F]Fluoroarenes by Nucleophilic Radiofluorination of Arylsulfonates. <i>Angewandte Chemie</i> , 2017, 129, 13186-13190.	2.0	10
94	Chiral Phosphoric Acid Dual-Function Catalysis: Asymmetric Allylation with β -Vinyl Allylboron Reagents. <i>Angewandte Chemie</i> , 2020, 132, 10627-10635.	2.0	10
95	Stereochemical Control via Chirality Pairing: Stereodivergent Syntheses of Enantioenriched Homoallylic Alcohols. <i>Angewandte Chemie</i> , 2021, 133, 24298-24308.	2.0	8
96	Stereodivergent Attached-Ring Synthesis via Non-Covalent Interactions: A Short Formal Synthesis of Merrilactone A. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	8
97	Theoretical enzyme design using the Kepler scientific workflows on the Grid. <i>Procedia Computer Science</i> , 2010, 1, 1175-1184.	2.0	7
98	Understanding the R882H mutation effects of DNA methyltransferase DNMT3A: a combination of molecular dynamics simulations and QM/MM calculations. <i>RSC Advances</i> , 2019, 9, 31425-31434.	3.6	7
99	Direct Synthesis of Ketones from Methyl Esters by Nickel-Catalyzed Suzuki-Miyaura Coupling. <i>Angewandte Chemie</i> , 2021, 133, 13588-13595.	2.0	7
100	Chiral Phosphoric Acid Catalyzed Conversion of Epoxides into Thiiranes: Mechanism, Stereochemical Model, and New Catalyst Design. <i>Angewandte Chemie</i> , 0, , .	2.0	6
101	Facilitating e-Science Discovery Using Scientific Workflows on the Grid. <i>Computer Communications and Networks</i> , 2011, , 353-382.	0.8	5
102	Cycloaddition Cascades of Strained Alkynes and Oxadiazinones. <i>Angewandte Chemie</i> , 2021, 133, 18349-18356.	2.0	4
103	Origins of Endo Selectivity in Diels-Alder Reactions of Cyclic Allene Dienophiles. <i>Angewandte Chemie</i> , 2021, 133, 15116-15124.	2.0	3
104	Control of Hetero-Diels-Alder Stereoselectivity through Solvent Polarity and Brønsted or Lewis Acid Catalysis; Theory and Experiment. <i>Synlett</i> , 2013, 24, 2446-2450.	1.8	2
105	Organic Chemistry and Synthesis Rely More and More upon Catalysts. <i>Catalysts</i> , 2022, 12, 758.	3.5	2
106	Rolf Huisgen's Classic Studies of Cyclic Triene Diels-Alder Reactions Elaborated by Modern Computational Analysis. <i>Angewandte Chemie</i> , 2020, 132, 12606-12619.	2.0	1
107	John D. Roberts, his beginnings at UCLA, his transformation of physical organic chemistry, and his impact on science. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3810.	1.9	0
108	Stereodivergent Attached-Ring Synthesis via Non-Covalent Interactions: A Short Formal Synthesis of Merrilactone A. <i>Angewandte Chemie</i> , 2022, 134, e202114514.	2.0	0