Donghui Wei

List of Publications by Year
in descending order

257 papers	9,679 citations	46918 47 h-index	53109 85 g-index
260 all docs	260 docs citations	260 times ranked	7232 citing authors

#	Article	IF	Citations
1	Non-fullerene acceptors with branched side chains and improved molecular packing to exceed 18% efficiency in organic solar cells. Nature Energy, 2021, 6, 605-613.	19.8	1,307
2	Highâ€Valentâ€Cobaltâ€Catalyzed Câ^'H Functionalization Based on Concerted Metalationâ€"Deprotonation and Singleâ€Electronâ€Transfer Mechanisms. ChemCatChem, 2016, 8, 1242-1263.	1.8	270
3	Alkyl Sideâ€Chain Engineering in Wideâ€Bandgap Copolymers Leading to Power Conversion Efficiencies over 10%. Advanced Materials, 2017, 29, 1604251.	11.1	213
4	Airâ€Stable, Leadâ€Free Zeroâ€Dimensional Mixed Bismuthâ€Antimony Perovskite Single Crystals with Ultraâ€broadband Emission. Angewandte Chemie - International Edition, 2019, 58, 2725-2729.	7.2	199
5	Colloidal Synthesis and Optical Properties of Allâ€Inorganic Lowâ€Dimensional Cesium Copper Halide Nanocrystals. Angewandte Chemie - International Edition, 2019, 58, 16087-16091.	7.2	192
6	Cooperative Multifunctional Organocatalysts for Ambient Conversion of Carbon Dioxide into Cyclic Carbonates. ACS Catalysis, 2018, 8, 9945-9957.	5.5	188
7	Copper-Catalyzed Direct Amination of Quinoline N-Oxides via Câ€"H Bond Activation under Mild Conditions. Organic Letters, 2014, 16, 1840-1843.	2.4	167
8	Leadâ€Free Sodiumâ€"Indium Double Perovskite Nanocrystals through Doping Silver Cations for Bright Yellow Emission. Angewandte Chemie - International Edition, 2019, 58, 17231-17235.	7.2	166
9	Mechanistic insights into cobalt(<scp>ii</scp>/<scp>iii</scp>)-catalyzed Câ€"H oxidation: a combined theoretical and experimental study. Chemical Science, 2015, 6, 7059-7071.	3.7	164
10	Tandem Silver Cluster Isomerism and Mixed Linkers to Modulate the Photoluminescence of Clusterâ€Assembled Materials. Angewandte Chemie - International Edition, 2018, 57, 8560-8566.	7.2	161
11	Organic Solar Cells Based on a 2D Benzo[1,2â€b:4,5â€bâ€²]difuranâ€Conjugated Polymer with Highâ€Power Conversion Efficiency. Advanced Materials, 2015, 27, 6969-6975.	11.1	151
12	A Crystalline Copper(II) Coordination Polymer for the Efficient Visibleâ€Lightâ€Driven Generation of Hydrogen. Angewandte Chemie - International Edition, 2016, 55, 2073-2077.	7.2	140
13	Efficient Thermally Activated Delayed Fluorescence from Allâ€Inorganic Cesium Zirconium Halide Perovskite Nanocrystals. Angewandte Chemie - International Edition, 2020, 59, 21925-21929.	7.2	126
14	A 1,8-Naphthyridine-Based Fluorescent Chemodosimeter for the Rapid Detection of Zn2+ and Cu2+. Organic Letters, 2008, 10, 5115-5118.	2.4	125
15	Silver-catalyzed decarboxylative radical cascade cyclization toward benzimidazo[2,1-a]isoquinolin-6(5H)-ones. Chemical Communications, 2019, 55, 2861-2864.	2.2	114
16	Cobalt(II)-Catalyzed Câ€"H Amination of Arenes with Simple Alkylamines. Organic Letters, 2016, 18, 1318-1321.	2.4	108
17	Recent Advances on Computational Investigations of Nâ€Heterocyclic Carbene Catalyzed Cycloaddition/Annulation Reactions: Mechanism and Origin of Selectivities. ChemCatChem, 2018, 10, 338-360.	1.8	106
18	Detection of Micro-Scale Li Dendrite via H2 Gas Capture for Early Safety Warning. Joule, 2020, 4, 1714-1729.	11.7	105

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19	Fundamental Reaction Pathway and Free Energy Profile for Inhibition of Proteasome by Epoxomicin. Journal of the American Chemical Society, 2012, 134, 10436-10450.	6.6	100
20	N-Heterocyclic Carbene (NHC)-Catalyzed sp³ Î²-Câ€“H Activation of Saturated Carbonyl Compounds: Mechanism, Role of NHC, and Origin of Stereoselectivity. ACS Catalysis, 2016, 6, 279-289.	5.5	99
21	Doped Zeroâ€Dimensional Cesium Zinc Halides for Highâ€Efficiency Blue Light Emission. Angewandte Chemie - International Edition, 2020, 59, 21414-21418.	7.2	97
22	Size effect of lead-free halide double perovskite on luminescence property. Science China Chemistry, 2019, 62, 1405-1413.	4.2	95
23	High Performance Organic Solar Cells Based on a Twisted Bayâ€Substituted Tetraphenyl Functionalized Perylenediimide Electron Acceptor. Advanced Energy Materials, 2015, 5, 1500032.	10.2	93
24	Direct regioselective phosphonation of heteroaryl N-oxides with H-phosphonates under metal and external oxidant free conditions. Chemical Communications, 2014, 50, 14409-14411.	2.2	84
25	Extension of indacenodithiophene backbone conjugation enables efficient asymmetric Aâ€“Dâ€“A type non-fullerene acceptors. Journal of Materials Chemistry A, 2018, 6, 18847-18852.	5.2	80
26	Colloidal Synthesis and Optical Properties of Allâ€Inorganic Lowâ€Dimensional Cesium Copper Halide Nanocrystals. Angewandte Chemie, 2019, 131, 16233-16237.	1.6	78
27	DFT perspective toward [3 + 2] annulation reaction of enals with Î±-ketoamides through NHC and BrÃ¸nsted acid cooperative catalysis: mechanism, stereoselectivity, and role of NHC. Organic Chemistry Frontiers, 2016, 3, 190-203.	2.3	74
28	Copper-Catalyzed Radical Cascade Cyclization To Access 3-Sulfonated Indenones with the AIE Phenomenon. Journal of Organic Chemistry, 2018, 83, 14419-14430.	1.7	74
29	Catalytic Mechanisms for Cofactor-Free Oxidase-Catalyzed Reactions: Reaction Pathways of Uricase-Catalyzed Oxidation and Hydration of Uric Acid. ACS Catalysis, 2017, 7, 4623-4636.	5.5	71
30	Organocatalytic asymmetric N-sulfonyl amide C-N bond activation to access axially chiral biaryl amino acids. Nature Communications, 2020, 11, 946.	5.8	71
31	Coupling of Ru and Oâ€Vacancy on 2D Moâ€Based Electrocatalyst Via a Solidâ€Phase Interface Reaction Strategy for Hydrogen Evolution Reaction. Advanced Energy Materials, 2021, 11, 2100141.	10.2	71
32	Peroxides as â€œSwitchesâ€• of Dialkyl H-Phosphonate: Two Mild and Metal-Free Methods for Preparation of 2-Acylbenzothiazoles and Dialkyl Benzothiazol-2-ylphosphonates. Journal of Organic Chemistry, 2014, 79, 8407-8416.	1.7	68
33	Insertion of chlorine atoms onto Ï€-bridges of conjugated polymer enables improved photovoltaic performance. Nano Energy, 2019, 58, 220-226.	8.2	67
34	A mitochondrial-targeted ratiometric probe for detecting intracellular H2S with high photostability. Chinese Chemical Letters, 2021, 32, 1799-1802.	4.8	65
35	Insights into the N-Heterocyclic Carbene (NHC)-Catalyzed Oxidative Î³-C(sp³)â€“H Deprotonation of Alkylenals and Cascade [4 + 2] Cycloaddition with Alkenylisoxazoles. Journal of Organic Chemistry, 2018, 83, 8543-8555.	1.7	61
36	Highâ€Valent Cobaltâ€Catalyzed Cî—¸H Activation/Annulation of 2â€Benzamidopyridine 1â€Oxide with Terminal Alkyne: A Combined Theoretical and Experimental Study. Advanced Synthesis and Catalysis, 2018, 360, 2668-2677.	2.1	61

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37	Reaction Pathway and Free Energy Profile for Papain-Catalyzed Hydrolysis of N-Acetyl-Phe-Gly 4-Nitroanilide. Biochemistry, 2013, 52, 5145-5154.	1.2	59
38	Insights into Stereoselective Aminomethylation Reaction of Î±,Î²-Unsaturated Aldehyde with N,O-Acetal via N-Heterocyclic Carbene and BrÃ¸nsted Acid/Base Cooperative Organocatalysis. Journal of Organic Chemistry, 2016, 81, 5370-5380.	1.7	59
39	Influence of reaction conditions on product distribution in the green oxidation of cyclohexene to adipic acid with hydrogen peroxide. Catalysis Today, 2011, 175, 619-624.	2.2	58
40	Theoretical Investigations toward the [4 + 2] Cycloaddition of Ketenes with N-Benzoyldiazenes Catalyzed by N-Heterocyclic Carbenes: Mechanism and Enantioselectivity. Journal of Organic Chemistry, 2012, 77, 10729-10737.	1.7	57
41	Lead-Free Small-Bandgap Cs₂CuSbCl₆ Double Perovskite Nanocrystals. Journal of Physical Chemistry Letters, 2020, 11, 6463-6467.	2.1	57
42	Computational Study on Î³-Câ€“H Functionalization of Î±,Î²-Unsaturated Ester Catalyzed by N-Heterocyclic Carbene: Mechanisms, Origin of Stereoselectivity, and Role of Catalyst. Journal of Organic Chemistry, 2017, 82, 13043-13050.	1.7	55
43	DFT Study on the Mechanisms and Stereoselectivities of the [4 + 2] Cycloadditions of Enals and Chalcones Catalyzed by N-Heterocyclic Carbene. Journal of Organic Chemistry, 2014, 79, 3069-3078.	1.7	52
44	Highly Enantioselective Catalytic System for Asymmetric Copolymerization of Carbon Dioxide and Cyclohexene Oxide. Chemistry - A European Journal, 2014, 20, 12394-12398.	1.7	51
45	Steric Engineering of Alkylthiolation Side Chains to Finely Tune Miscibility in Nonfullerene Polymer Solar Cells. Advanced Energy Materials, 2019, 9, 1802686.	10.2	51
46	Prediction on the origin of selectivities of NHC-catalyzed asymmetric dearomatization (CADA) reactions. Catalysis Science and Technology, 2019, 9, 465-476.	2.1	50
47	Insights into N-heterocyclic carbene-catalyzed [3 + 4] annulation reactions of 2-bromoenals with N-Ts hydrazones. Organic Chemistry Frontiers, 2018, 5, 2739-2748.	2.3	49
48	Atroposelective isoquinolinone synthesis through cobalt-catalysed Câ€“H activation and annulation. , 2022, 1, 709-718.		49
49	A quantum mechanical study of the mechanism and stereoselectivity of the N-heterocyclic carbene catalyzed [4 + 2] annulation reaction of enals with azodicarboxylates. Organic Chemistry Frontiers, 2015, 2, 874-884.	2.3	48
50	Insights into NHC-catalyzed oxidative Î±-C(sp³)â€“H activation of aliphatic aldehydes and cascade [2 + 3] cycloaddition with azomethine imines. Catalysis Science and Technology, 2019, 9, 2514-2522.	2.1	48
51	Computational study on NHC-catalyzed enantioselective and chemoselective fluorination of aliphatic aldehydes. Organic Chemistry Frontiers, 2017, 4, 1987-1998.	2.3	47
52	A DFT study on enantioselective synthesis of aza-Î²-lactams via NHC-catalyzed [2+2] cycloaddition of ketenes with diazenedicarboxylates. Journal of Molecular Catalysis A, 2011, 334, 108-115.	4.8	46
53	DFT Study on the Mechanisms and Diastereoselectivities of Lewis Acid-Promoted Keteneâ€“Alkene [2 + 2] Cycloadditions: What is the Role of Lewis Acid in the Ketene and C = X (X = O, CH₂, and NH) [2 + 2] Cycloaddition Reactions?. Journal of Physical Chemistry A, 2014, 118, 4288-4300.	1.1	46
54	Prediction of NHC-catalyzed chemoselective functionalizations of carbonyl compounds: a general mechanistic map. Chemical Science, 2020, 11, 7214-7225.	3.7	44

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55	Prediction on the Origin of Selectivities in Baseâ€controlled Switchable NHCâ€catalyzed Transformations. Chemistry - an Asian Journal, 2019, 14, 293-300.	1.7	42
56	Insights into N-Heterocyclic Carbene-Catalyzed Oxidative Î±-C(sp³)â€“H Activation of Aliphatic Aldehydes and Cascade [2 + 2] Cycloaddition with Ketimines. Journal of Organic Chemistry, 2019, 84, 6117-6125.	1.7	42
57	NHC-Catalyzed Aldol-Like Reactions of Allenoates with Isatins: Regiospecific Syntheses of Î³-Functionalized Allenoates. Organic Letters, 2019, 21, 1306-1310.	2.4	42
58	Nonâ€Fullerene Organic Solar Cells Based on Benzo[1,2â€b:4,5â€bâ€²]difuranâ€Conjugated Polymer with 14% Efficiency. Advanced Functional Materials, 2020, 30, 1906809.	7.8	41
59	Competing mechanisms and origins of chemo- and stereo-selectivities of NHC-catalyzed reactions of enals with 2-aminoacrylates. Catalysis Science and Technology, 2018, 8, 4229-4240.	2.1	40
60	Atroposelective Synthesis of Axially Chiral 4-Aryl Î±-Carbolines via N-Heterocyclic Carbene Catalysis. Organic Letters, 2021, 23, 4267-4272.	2.4	40
61	Asymmetric Carbeneâ€Catalyzed Oxidation of Functionalized Aldimines as 1,4â€Dipoles. Angewandte Chemie - International Edition, 2021, 60, 7913-7919.	7.2	39
62	DFT Investigation on Mechanisms and Stereoselectivities of [2 + 2 + 2] Multimolecular Cycloaddition of Ketenes and Carbon Disulfide Catalyzed by N-Heterocyclic Carbenes. Journal of Organic Chemistry, 2013, 78, 11849-11859.	1.7	38
63	A DFT study on NHC-catalyzed intramolecular aldehydeâ€“ketone crossed-benzoin reaction: mechanism, regioselectivity, stereoselectivity, and role of NHC. Organic and Biomolecular Chemistry, 2016, 14, 6577-6590.	1.5	38
64	Insights into highly selective ring expansion of oxaziridines under Lewis base catalysis: a DFT study. Organic Chemistry Frontiers, 2019, 6, 679-687.	2.3	38
65	Multiple Functional Organocatalyst-Promoted Inert Câ€“C Activation: Mechanism and Origin of Selectivities. ACS Catalysis, 2021, 11, 3443-3454.	5.5	38
66	Insights into the Unexpected Chemoselectivity for the N-Heterocyclic Carbene-Catalyzed Annulation Reaction of Allenals with Chalcones. Journal of Organic Chemistry, 2015, 80, 8619-8630.	1.7	37
67	Fundamental Reaction Pathway for Peptide Metabolism by Proteasome: Insights from First-Principles Quantum Mechanical/Molecular Mechanical Free Energy Calculations. Journal of Physical Chemistry B, 2013, 117, 13418-13434.	1.2	36
68	DFT study on the reaction mechanisms and stereoselectivities of NHC-catalyzed [2 + 2] cycloaddition between arylalkylketenes and electron-deficient benzaldehydes. Organic and Biomolecular Chemistry, 2014, 12, 6374.	1.5	36
69	Mechanisms and stereoselectivities of the Rh(<scp>i</scp>)-catalyzed carbenoid carbon insertion reaction of benzocyclobutenol with diazoester. Organic and Biomolecular Chemistry, 2015, 13, 6587-6597.	1.5	36
70	A computational study on the N-heterocyclic carbene-catalyzed C_{sp2}â€“C_{sp3} bond activation/[4+2] cycloaddition cascade reaction of cyclobutenones with imines: a new application of the conservation principle of molecular orbital symmetry. Physical Chemistry Chemical Physics, 2016, 18, 19933-19943.	1.3	36
71	Leadâ€Free Sodiumâ€“Indium Double Perovskite Nanocrystals through Doping Silver Cations for Bright Yellow Emission. Angewandte Chemie, 2019, 131, 17391-17395.	1.6	36
72	Manganese Catalyzed Direct Amidation of Esters with Amines. Journal of Organic Chemistry, 2021, 86, 2339-2358.	1.7	36

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73	Insights into the NHC-catalyzed cascade Michael/aldol/lactamization reaction: mechanism and origin of stereoselectivity. Organic Chemistry Frontiers, 2018, 5, 2065-2072.	2.3	35
74	Insights into the Oxidative Palladiumâ€Catalyzed Regioselective Synthesis of 3â€Arylindoles from Nâ^Tsâ€Anilines and Styrenes: A Computational Study. ChemCatChem, 2019, 11, 780-789.	1.8	35
75	A Multiheteroatom [3,3]-Sigmatropic Rearrangement: Disproportionative Entries into 2-(N-Heteroaryl)methyl Phosphates and Î±-Keto Phosphates. Organic Letters, 2017, 19, 5864-5867.	2.4	34
76	Insights into the Nâ€Heterocyclic Carbene (NHC)â€Catalyzed Intramolecular Cyclization of Aldimines: General Mechanism and Role of Catalyst. Chemistry - an Asian Journal, 2018, 13, 1710-1718.	1.7	34
77	Asymmetric Aâ€“Dâ€“Ïâ€“A-type nonfullerene small molecule acceptors for efficient organic solar cells. Journal of Materials Chemistry A, 2019, 7, 19348-19354.	5.2	33
78	Insights into Nâ€Heterocyclic Carbeneâ€Catalyzed [4+2] Annulation Reaction of Enals with Nitroalkenes: Mechanisms, Origin of Chemoâ€•and Stereoselectivity, and Role of Catalyst. Chemistry - an Asian Journal, 2016, 11, 3046-3054.	1.7	32
79	A DFT study on PBu₃-catalyzed intramolecular cyclizations of N-allylic substituted Î±-amino nitriles for the formation of functionalized pyrrolidines: mechanisms, selectivities, and the role of catalysts. Organic and Biomolecular Chemistry, 2016, 14, 3130-3141.	1.5	32
80	Mitochondria-dependent benzothiadiazole-based molecule probe for quantitatively intracellular pH imaging. Dyes and Pigments, 2017, 145, 576-583.	2.0	32
81	High-efficiency organic solar cells enabled by an alcohol-washable solid additive. Science China Chemistry, 2021, 64, 2161-2168.	4.2	32
82	Iridium(<scp>iii</scp>) complexes bearing oxadiazol-substituted amide ligands: color tuning and application in highly efficient phosphorescent organic light-emitting diodes. Journal of Materials Chemistry C, 2017, 5, 9146-9156.	2.7	31
83	Insights into the isothiourea-catalyzed asymmetric [4 + 2] annulation of phenylacetic acid with alkylidene pyrazolone. Organic and Biomolecular Chemistry, 2018, 16, 2301-2311.	1.5	31
84	Recycling of silicon from silicon cutting waste by Al-Si alloying in cryolite media and its mechanism analysis. Environmental Pollution, 2020, 265, 114892.	3.7	30
85	Insight into the organocatalytic arylation of azonaphthalenes with Î±-chloroaldehydes: the general mechanism and origin of selectivities. Chemical Communications, 2021, 57, 219-222.	2.2	29
86	Diradical Generation via Relayed Proton-Coupled Electron Transfer. Journal of the American Chemical Society, 2022, 144, 3137-3145.	6.6	29
87	Fundamental reaction pathway and free energy profile of proteasome inhibition by syringolin A (SylA). Organic and Biomolecular Chemistry, 2015, 13, 6857-6865.	1.5	28
88	DFT Study on the Mechanism and Stereoselectivity of NHC-Catalyzed Synthesis of Substituted Trifluoromethyl Dihydropyranones with Contiguous Stereocenters. Journal of Organic Chemistry, 2016, 81, 868-877.	1.7	28
89	High efficiency non-fullerene organic solar cells without electron transporting layers enabled by Lewis base anion doping. Nano Energy, 2018, 51, 736-744.	8.2	28
90	Predicting the origin of selectivity in NHC-catalyzed ring opening of formylcyclopropane: a theoretical investigation. Catalysis Science and Technology, 2021, 11, 332-337.	2.1	28

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91	A theoretical study on the mechanisms of the reactions between 1,3-diallkynes and ammonia derivatives for the formation of five-membered N-heterocycles. Organic and Biomolecular Chemistry, 2014, 12, 7503-7514.	1.5	27
92	Origin of Regioâ€•and Stereoselectivity in the NHCâ€catalyzed Reaction of Alkyl Pyridinium with Aliphatic Enal. ChemCatChem, 2020, 12, 1068-1074.	1.8	27
93	Highly Active and Robust Ruthenium Complexes Based on Hemilability of Hybrid Ligands for Câ€“H Oxidation. Journal of Organic Chemistry, 2020, 85, 4324-4334.	1.7	27
94	A DFT study of the enantioselective reduction of prochiral ketones promoted by pinene-derived amino alcohols. Tetrahedron: Asymmetry, 2009, 20, 1020-1026.	1.8	26
95	Influence of aromatic heterocycle of conjugated side chains on photovoltaic performance of benzodithiophene-based wide-bandgap polymers. Polymer Chemistry, 2016, 7, 4036-4045.	1.9	26
96	Synthesis and properties of benzothiadiazole-pyridine system: TheÂmodulation of optical feature. Dyes and Pigments, 2017, 137, 135-142.	2.0	26
97	Theoretical study on the mechanism and enantioselectivity of NHC-catalyzed intramolecular S_N2â€² nucleophilic substitution: what are the roles of NHC and DBU?. Organic Chemistry Frontiers, 2018, 5, 1493-1501.	2.3	26
98	Two Birds with One Stone: High Efficiency and Low Synthetic Cost for Benzotriazoleâ€Based Polymer Solar Cells by a Simple Chemical Approach. Advanced Energy Materials, 2020, 10, 2002142.	10.2	26
99	Unveiling the Chemo- and Stereoselectivities of NHC-Catalyzed Reactions of an Aliphatic Ester with Aminochalcone. Journal of Organic Chemistry, 2020, 85, 8437-8446.	1.7	26
100	Theoretical Model for N-Heterocyclic Carbene-Catalyzed Desymmetrizing [4 + 1] and [4 + 2] Annulations of an Enal and Aryldialdehyde with 1,3-Cyclopentenedione. Organic Letters, 2021, 23, 2421-2425.	2.4	26
101	DFT Study on the Mechanisms of Stereoselective C(2)-Vinylation of 1-Substituted Imidazoles with 3-Phenyl-2-propynenitrile. Journal of Physical Chemistry A, 2009, 113, 11035-11041.	1.1	25
102	Theoretical Investigations toward the Asymmetric Insertion Reaction of Diazoester with Aldehyde Catalyzed by N-Protonated Chiral Oxazaborolidine: Mechanisms and Stereoselectivity. Journal of Physical Chemistry A, 2015, 119, 8422-8431.	1.1	25
103	With metal or not? a computationally predicted rule for a dirhodium catalyst in [3+3] cycloadditions of triazole with thiirane. Chemical Communications, 2020, 56, 4732-4735.	2.2	25
104	Insights into N-heterocyclic carbene and Lewis acid cooperatively catalyzed oxidative [3 + 3] annulation reactions of Î±,Î²-unsaturated aldehyde with 1,3-dicarbonyl compounds. Organic Chemistry Frontiers, 2020, 7, 1113-1121.	2.3	25
105	Asymmetric Carbeneâ€Catalyzed Oxidation of Functionalized Aldimines as 1,4â€Dipoles. Angewandte Chemie, 2021, 133, 7992-7998.	1.6	25
106	Highly Stereo-Controlled Synthesis of Fatty Acid-Derived Cyclic Carbonates by Using Iron(II) Complex and Nucleophilic Halide. Journal of Organic Chemistry, 2019, 84, 11407-11416.	1.7	24
107	Efficient Thermally Activated Delayed Fluorescence from Allâ€Inorganic Cesium Zirconium Halide Perovskite Nanocrystals. Angewandte Chemie, 2020, 132, 22109-22113.	1.6	24
108	Prediction on the origin of chemoselectivity in Lewis base-mediated competition cyclizations between allenoates and chalcones: a computational study. Organic Chemistry Frontiers, 2019, 6, 2692-2700.	2.3	23

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109	Mechanisms of the cascade synthesis of substituted 4â€aminoâ€1,2,4â€triazolâ€3â€one from huisgen zwitterion and aldehyde hydrazone: A DFT study. Journal of Computational Chemistry, 2012, 33, 715-722.	1.5	22
110	Neutral and Cationic NCN Pincer Platinum(II) Complexes with 1,3-Bis(benzimidazol-2â€²-yl)benzene Ligands: Synthesis, Structures, and Their Photophysical Properties. Organometallics, 2014, 33, 1563-1573.	1.1	22
111	Effects of Intercalated Molecules in Graphene Oxide on the Interlayer Channels for Anhydrous Proton Conduction. Industrial & Engineering Chemistry Research, 2016, 55, 11931-11942.	1.8	22
112	High-performance wide-bandgap copolymers based on indacenodithiophene and indacenodithieno[3,2-b]thiophene units. Journal of Materials Chemistry C, 2017, 5, 7777-7783.	2.7	22
113	Theoretical investigations of the Ir-catalyzed direct borylation of B(3,6)â€“H of o-carborane: the actual catalyst, mechanism, and origin of regioselectivity. Catalysis Science and Technology, 2018, 8, 5165-5177.	2.1	22
114	Substitution Dependent Ultrafast Ultraviolet Energy Dissipation Mechanisms of Plant Sunscreens. Journal of Physical Chemistry Letters, 2019, 10, 5244-5249.	2.1	22
115	Hydroboration Reaction and Mechanism of Carboxylic Acids using NaNH₂(BH₃)₂, a Hydroboration Reagent with Reducing Capability between NaBH₄ and LiAlH₄. Journal of Organic Chemistry, 2021, 86, 5305-5316.	1.7	22
116	A DFT study on the reaction mechanisms of keteneâ€“ketone [2+2+2] cycloaddition to form 3-aryglutaric anhydrides under a Lewis acid catalysis: What is the role of BF3?. Journal of Molecular Catalysis A, 2010, 326, 41-47.	4.8	21
117	A DFT study on the reaction mechanism of dimerization of methyl methacrylate catalyzed by N-heterocyclic carbene. Physical Chemistry Chemical Physics, 2014, 16, 20001-20008.	1.3	21
118	Regioselective Synthesis of Sulfonyl-Containing Benzyl Dithiocarbamates through Copper-Catalyzed Thiosulfonylation of Styrenes. Journal of Organic Chemistry, 2019, 84, 11135-11149.	1.7	21
119	Theoretical Study on the Reaction Mechanism between 6-Benzyl-6-azabicyclo[2.2.1]hept-2-ene and Benzoyl Isocyanate to Urea and Isourea. Journal of Physical Chemistry A, 2010, 114, 2913-2919.	1.1	20
120	Theoretical investigations toward TMEDA-catalyzed [2 + 4] annulation of allenoate with 1-aza-1,3-diene: mechanism, regioselectivity, and role of the catalyst. RSC Advances, 2016, 6, 70723-70731.	1.7	20
121	Unique structural micro-adjustments in a new benzothiadiazole-derived Zn(<scp>ii</scp>) metal organic framework via simple photochemical decarboxylation. Chemical Communications, 2017, 53, 10314-10317.	2.2	20
122	Unravelling a general mechanism of converting ionic B/N complexes into neutral B/N analogues of alkanes: H^{Î´+}â‹¯H^{Î´â€“} dihydrogen bonding assisted dehydrogenation. Chemical Communications, 2019, 55, 12239-12242.	2.2	20
123	Unravelling the Mechanism and Selectivity of the NHCâ€catalyzed Threeâ€Membered Ringâ€Opening/Fluorination of Epoxy Enals: A DFT Study. ChemCatChem, 2019, 11, 2919-2925.	1.8	20
124	Insights into Nâ€Heterocyclic Carbene (NHC)â€Catalyzed Asymmetric Addition of 2Hâ€Azirine with Aldehyde. Chemistry - an Asian Journal, 2019, 14, 2000-2007.	1.7	20
125	Binuclear Tridentate Hemilabile Copper(I) Catalysts for Utilization of CO₂ into Oxazolidinones from Propargylic Amines. Journal of Organic Chemistry, 2020, 85, 15197-15212.	1.7	20
126	Copper(<scp>i</scp>)/Ganphos catalysis: enantioselective synthesis of diverse spirooxindoles using iminoesters and alkyl substituted methyleneindolinones. Organic and Biomolecular Chemistry, 2020, 18, 3740-3746.	1.5	20

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127	Insights into the chiral sulfide/selenide-catalyzed electrophilic carbothiolation of alkynes: mechanism and origin of axial chirality. Organic Chemistry Frontiers, 2021, 8, 1983-1990.	2.3	20
128	A combined experimental and DFT study of active structures and self-cycle mechanisms of mononuclear tungsten peroxo complexes in oxidation reactions. Journal of Molecular Structure, 2011, 992, 19-26.	1.8	19
129	Direct diphosphonylation of quinolines with H-phosphonates under metal-free conditions. Tetrahedron, 2015, 71, 6087-6093.	1.0	19
130	Insights into the Competing Mechanisms and Origin of Enantioselectivity for N-Heterocyclic Carbene-Catalyzed Reaction of Aldehyde with Enamide. Scientific Reports, 2016, 6, 38200.	1.6	19
131	A DFT Study on Mechanisms and Origin of Selectivity of Phosphine-Catalyzed Vicinal Acylcyanation of Alkynoates. ChemistrySelect, 2017, 2, 5266-5273.	0.7	19
132	Schiff-based Pd(II)/Fe(III) bimetallic self-assembly monolayer---preparation, structure, catalytic dynamic and synergistic. Molecular Catalysis, 2019, 469, 75-86.	1.0	19
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