Xiaotian Qi

List of Publications by Year
in descending order

89 papers	4,216 citations	101543 36 h-index	123424 61 g-index
91 all docs	91 docs citations	91 times ranked	3551 citing authors

#	Article	IF	Citations
1	From Esters to Ketones via a Photoredoxâ€Assisted Reductive Acyl Crossâ€Coupling Strategy. Angewandte Chemie - International Edition, 2022, 61, .	13.8	28
2	From Esters to Ketones via a Photoredoxâ€Assisted Reductive Acyl Crossâ€Coupling Strategy. Angewandte Chemie, 2022, 134, .	2.0	5
3	Photoredox-Enabled Chromium-Catalyzed Alkene Diacylations. ACS Catalysis, 2022, 12, 1879-1885.	11.2	32
4	Precise electro-reduction of alkyl halides for radical defluorinative alkylation. Science China Chemistry, 2022, 65, 762-770.	8.2	31
5	Chemical Recycling of Polystyrene to Valuable Chemicals via Selective Acid-Catalyzed Aerobic Oxidation under Visible Light. Journal of the American Chemical Society, 2022, 144, 6532-6542.	13.7	111
6	ProPhenol Derived Ligands to Simultaneously Coordinate a Mainâ€Group Metal and a Transition Metal: Application to a Znâˆ'Cu Catalyzed Reaction. Chemistry - A European Journal, 2022, 28, e202104268.	3.3	10
7	Epoxide Electroreduction. Journal of the American Chemical Society, 2022, 144, 1389-1395.	13.7	42
8	Diastereoselective Transfer of Tri(di)fluoroacetylsilanesâ€Derived Carbenes to Alkenes. Angewandte Chemie - International Edition, 2022, 61, .	13.8	43
9	Diastereoselective Transfer of Tri(di)fluoroacetylsilanesâ€Derived Carbenes to Alkenes. Angewandte Chemie, 2022, 134, .	2.0	7
10	Visual Kinetic Analysis and Quantum Chemical Calculations Uncover the Mechanistic Insights into Rh-Catalyzed [5+2+1] Cycloaddition. Chinese Journal of Organic Chemistry, 2022, 42, 1258.	1.3	1
11	Dual-resolving of positional and geometric isomers of C=C bonds via bifunctional photocycloaddition-photoisomerization reaction system. Nature Communications, 2022, 13, 2652.	12.8	18
12	Ligand Conformational Flexibility Enables Enantioselective Tertiary Câ€"B Bond Formation in the Phosphonate-Directed Catalytic Asymmetric Alkene Hydroboration. Journal of the American Chemical Society, 2021, 143, 4801-4808.	13.7	30
13	Enantioselective Synthesis of Î±-All-Carbon Quaternary Center-Containing Carbazolones via Amino-palladation/Desymmetrizing Nitrile Addition Cascade. Journal of the American Chemical Society, 2021, 143, 3734-3740.	13.7	37
14	Stereoselective Palladium-Catalyzed Base-Free Suzukiâ€"Miyaura Cross-Coupling of Tetrasubstituted <i>gem</i>-Difluoroalkenes: An Experimental and Computational Study. ACS Catalysis, 2021, 11, 4799-4809.	11.2	52
15	Energy Decomposition Analysis Reveals the Nature of Lone Pairâˆ'Ï€ Interactions with Cationic Ï€ Systems in Catalytic Acyl Transfer Reactions. Organic Letters, 2021, 23, 4411-4414.	4.6	12
16	Tandem Iridium Catalysis as a General Strategy for Atroposelective Construction of Axially Chiral Styrenes. Journal of the American Chemical Society, 2021, 143, 10686-10694.	13.7	71
17	Recent Advances in Theoretical Studies on Transition-Metal-Catalyzed Carbene Transformations. Accounts of Chemical Research, 2021, 54, 2905-2915.	15.6	60
18	Development and Mechanistic Studies of the Iridiumâ€Catalyzed Câˆ'H Alkenylation of Enamides with Vinyl Acetates: A Versatile Approach for Ketone Functionalization. Angewandte Chemie, 2021, 133, 21094-21102.	2.0	2

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19	Development and Mechanistic Studies of the Iridiumâ€Catalyzed Câˆ’H Alkenylation of Enamides with Vinyl Acetates: A Versatile Approach for Ketone Functionalization. Angewandte Chemie - International Edition, 2021, 60, 20926-20934.	13.8	12
20	Electrochemical Borylation of Alkyl Halides: Fast, Scalable Access to Alkyl Boronic Esters. Journal of the American Chemical Society, 2021, 143, 12985-12991.	13.7	65
21	P-stereogenic N-vinylphosphonamides enabled by asymmetric allylic substitution-isomerization. Cell Reports Physical Science, 2021, 2, 100594.	5.6	14
22	Time-Resolved EPR Revealed the Formation, Structure, and Reactivity of N<i>-</i>Centered Radicals in an Electrochemical C(sp³)â€“H Arylation Reaction. Journal of the American Chemical Society, 2021, 143, 20863-20872.	13.7	64
23	Compatibility Score for Rational Electrophile Selection in Pd/NBE Cooperative Catalysis. CheM, 2020, 6, 2810-2825.	11.7	22
24	Application of Trimethylgermanyl-Substituted Bisphosphine Ligands with Enhanced Dispersion Interactions to Copper-Catalyzed Hydroboration of Disubstituted Alkenes. Journal of the American Chemical Society, 2020, 142, 18213-18222.	13.7	73
25	Asymmetric allylic substitutionâ€“isomerization to axially chiral enamides <i>via</i> hydrogen-bonding assisted central-to-axial chirality transfer. Chemical Science, 2020, 11, 10119-10126.	7.4	57
26	Stereodivergent Alkyne Hydrofluorination Using Protic Tetrafluoroborates as Tunable Reagents. Angewandte Chemie - International Edition, 2020, 59, 16651-16660.	13.8	34
27	<i>Î²</i>â€Mannosylation through <i>O</i>â€Alkylation of Anomeric Cesium Alkoxides: Mechanistic Studies and Synthesis of the Hexasaccharide Core of Complex Fucosylated Nâ€Linked Glycans. European Journal of Organic Chemistry, 2020, 2020, 2291-2301.	2.4	13
28	Stereodivergent Alkyne Hydrofluorination Using Protic Tetrafluoroborates as Tunable Reagents. Angewandte Chemie, 2020, 132, 16794.	2.0	6
29	2-Sulfonylpyridines as Tunable, Cysteine-Reactive Electrophiles. Journal of the American Chemical Society, 2020, 142, 8972-8979.	13.7	64
30	An enzymatic platform for the asymmetric amination of primary, secondary and tertiary C(sp3)â€“H bonds. Nature Chemistry, 2019, 11, 987-993.	13.6	146
31	Theoretical study of the ligand effect on NHCâ€“cobalt-catalyzed hydrogenation of ketones. Catalysis Science and Technology, 2019, 9, 5315-5321.	4.1	6
32	Branchedâ€Selective Direct Î±â€Alkylation of Cyclic Ketones with Simple Alkenes. Angewandte Chemie - International Edition, 2019, 58, 4366-4370.	13.8	53
33	Revealing the reduction process of Cu(<scp>ii</scp>) by sodium bis(trimethylsilyl)amide. Faraday Discussions, 2019, 220, 105-112.	3.2	5
34	Energy Decomposition Analyses Reveal the Origins of Catalyst and Nucleophile Effects on Regioselectivity in Nucleopalladation of Alkenes. Journal of the American Chemical Society, 2019, 141, 11892-11904.	13.7	61
35	Deacylative transformations of ketones via aromatization-promoted Câ€“C bond activation. Nature, 2019, 567, 373-378.	27.8	135
36	Branchedâ€Selective Direct Î±â€Alkylation of Cyclic Ketones with Simple Alkenes. Angewandte Chemie, 2019, 131, 4410-4414.	2.0	14

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37	Theoretical Study of Ni-Catalyzed Câ€“N Radicalâ€“Radical Cross-Coupling. Journal of Organic Chemistry, 2019, 84, 3321-3327.	3.2	18
38	Site-Selective and Stereoselective <i>O</i>-Alkylation of Glycosides by Rh(II)-Catalyzed Carbenoid Insertion. Journal of the American Chemical Society, 2019, 141, 19902-19910.	13.7	36
39	Mechanistic insight into cobalt-catalyzed stereodivergent semihydrogenation of alkynes: The story of selectivity control. Journal of Catalysis, 2018, 362, 25-34.	6.2	55
40	Câ€“H bond cleavage occurring on a Rh(<scp>v</scp>) intermediate: a theoretical study of Rh-catalyzed arene azidation. Catalysis Science and Technology, 2018, 8, 1645-1651.	4.1	35
41	Insights into disilylation and distannation: sequence influence and ligand/steric effects on Pd-catalyzed difunctionalization of carbenes. Dalton Transactions, 2018, 47, 1819-1826.	3.3	21
42	The mechanism of copper-catalyzed oxytrifluoromethylation of allylamines with CO₂: a computational study. Organic Chemistry Frontiers, 2018, 5, 633-639.	4.5	46
43	Long distance unconjugated agostic-assisted 1,5-H shift in a Ru-mediated Alder-ene type reaction: mechanism and stereoselectivity. Organic Chemistry Frontiers, 2018, 5, 3178-3185.	4.5	13
44	Revealing the Structure and Reactivity of the Active Species in the FeCl₂â€“TBHP System: Case Study on Alkene Oxidation. Organometallics, 2018, 37, 1635-1640.	2.3	7
45	Thiolateâ€“palladium(<scp>iv</scp>) or sulfoniumâ€“palladate(0)? A theoretical study on the mechanism of palladium-catalyzed Câ€“S bond formation reactions. Organic Chemistry Frontiers, 2017, 4, 943-950.	4.5	13
46	Mononuclear or Dinuclear? Mechanistic Study of the Zincâ€Catalyzed Oxidative Coupling of Aldehydes and Acetylenes. Chemistry - A European Journal, 2017, 23, 6419-6425.	3.3	18
47	Mechanism, Regio-, and Diastereoselectivity of Rh(III)-Catalyzed Cyclization Reactions of <i>N</i>-Arylnitrones with Alkynes: A Density Functional Theory Study. Journal of Physical Chemistry A, 2017, 121, 4496-4504.	2.5	17
48	Visibleâ€Lightâ€Driven Azaâ€<i>ortho</i>â€quinone Methide Generation for the Synthesis of Indoles in a Multicomponent Reaction. Angewandte Chemie - International Edition, 2017, 56, 9527-9531.	13.8	125
49	Visibleâ€Lightâ€Driven Azaâ€<i>ortho</i>â€quinone Methide Generation for the Synthesis of Indoles in a Multicomponent Reaction. Angewandte Chemie, 2017, 129, 9655-9659.	2.0	31
50	Coordination strategy-induced selective Câ€“H amination of 8-aminoquinolines. Chemical Communications, 2017, 53, 6736-6739.	4.1	34
51	Ir(III)/Ir(V) or Ir(I)/Ir(III) Catalytic Cycle? Steric-Effect-Controlled Mechanism for the <i>para</i>-Câ€“H Borylation of Arenes. Organometallics, 2017, 36, 2107-2115.	2.3	38
52	Stabilization of Two Radicals with One Metal: A Stepwise Coupling Model for Copper-Catalyzed Radicalâ€“Radical Cross-Coupling. Scientific Reports, 2017, 7, 43579.	3.3	35
53	Room-Temperature Coupling/Decarboxylation Reaction of Î±-Oxocarboxylates with Î±-Bromoketones: Solvent-Controlled Regioselectivity for 1,2- and 1,3-Diketones. Journal of Organic Chemistry, 2017, 82, 1403-1411.	3.2	22
54	Computational Investigation of the Role Played by Rhodium(V) in the Rhodium(III)â€Catalyzed <i>ortho</i>â€Bromination of Arenes. Chemistry - A European Journal, 2017, 23, 2690-2699.	3.3	32

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55	Bond dissociation energy controlled Ïƒ-bond metathesis in alkaline-earth-metal hydride catalyzed dehydrocoupling of amines and boranes: a theoretical study. Inorganic Chemistry Frontiers, 2017, 4, 1813-1820.	6.0	18
56	From Mechanistic Study to Chiral Catalyst Optimization: Theoretical Insight into Binaphthophosphepine-catalyzed Asymmetric Intramolecular [3 + 2] Cycloaddition. Scientific Reports, 2017, 7, 7619.	3.3	11
57	Mechanism of Rhodium-Catalyzed Câ€“H Functionalization: Advances in Theoretical Investigation. Accounts of Chemical Research, 2017, 50, 2799-2808.	15.6	203
58	Oxidation-induced Câ€“H amination leads to a new avenue to build Câ€“N bonds. Chemical Communications, 2017, 53, 8984-8987.	4.1	16
59	Readily Accessible and Highly Efficient Ferroceneâ€Based Aminoâ€Phosphineâ€Alcohol (fâ€Amphol) Ligands for Iridiumâ€Catalyzed Asymmetric Hydrogenation of Simple Ketones. Chemistry - A European Journal, 2017, 23, 970-975.	3.3	67
60	Ligand effect on nickle-catalyzed reductive alkyne-aldehyde coupling reactions: a computational study. Scientia Sinica Chimica, 2017, 47, 341-349.	0.4	2
61	Mechanistic insights into copper-catalyzed trifluoromethylation of aryl boronic acids: a theoretical study. Scientia Sinica Chimica, 2017, 47, 859-864.	0.4	3
62	Mechanism of Ruthenium-Catalyzed Direct Arylation of Câ€“H Bonds in Aromatic Amides: A Computational Study. Organometallics, 2016, 35, 1440-1445.	2.3	39
63	Radicalâ€“Radical Cross-Coupling for Câ€“S Bond Formation. Organic Letters, 2016, 18, 2351-2354.	4.6	78
64	Computational Studies on an Aminomethylation Precursor: (Xantphos)Pd(CH₂NBn₂)⁺. Organometallics, 2016, 35, 1582-1585.	2.3	14
65	Homolytic cleavage of the Oâ€“Cu(<scp>ii</scp>) bond: XAFS and EPR spectroscopy evidence for one electron reduction of Cu(<scp>ii</scp>) to Cu(<scp>i</scp>). Chemical Communications, 2016, 52, 6914-6917.	4.1	25
66	Aromatic Câ€“H bond cleavage by using a Cu(i) ate-complex. Organic Chemistry Frontiers, 2016, 3, 975-978.	4.5	6
67	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.	3.3	21
68	Effective Chirality Transfer in [3+2] Reaction between Allenyl-Rhodium and Enal: Mechanistic Study Based on DFT Calculations. Journal of Organic Chemistry, 2016, 81, 8306-8311.	3.2	15
69	Catalytic N-radical cascade reaction of hydrazones by oxidative deprotonation electron transfer and TEMPO mediation. Nature Communications, 2016, 7, 11188.	12.8	196
70	Mechanism of Synergistic Cu(II)/Cu(I)-Mediated Alkyne Coupling: Dinuclear 1,2-Reductive Elimination after Minimum Energy Crossing Point. Journal of Organic Chemistry, 2016, 81, 1654-1660.	3.2	42
71	Rhodium-Catalyzed Hetero-(5 + 2) Cycloaddition of Vinylaziridines and Alkynes: A Theoretical View of the Mechanism and Chirality Transfer. Organometallics, 2016, 35, 771-777.	2.3	33
72	Mechanism, chemoselectivity and enantioselectivity for the rhodium-catalyzed desymmetric synthesis of hydrobenzofurans: a theoretical study. Organic Chemistry Frontiers, 2016, 3, 209-216.	4.5	21

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73	Tuning the Reactivity of Radical through a Triplet Diradical Cu(II) Intermediate in Radical Oxidative Cross-Coupling. Scientific Reports, 2015, 5, 15934.	3.3	34
74	The Mechanism of Nï£¿O Bond Cleavage in Rhodiumâ€Catalyzed Cï£¿H Bond Functionalization of Quinoline <i>N</i>â€oxides with Alkynes: A Computational Study. Chemistry - A European Journal, 2015, 21, 10131-10137.	3.3	59
75	Mechanism and selectivity for zinc-mediated cycloaddition of azides with alkynes: a computational study. RSC Advances, 2015, 5, 49802-49808.	3.6	23
76	Nickel-Catalyzed Selective Oxidative Radical Cross-Coupling: AnÂEffective Strategy for Inert Csp³â€“H Functionalization. Organic Letters, 2015, 17, 998-1001.	4.6	76
77	Tuning radical reactivity using iodine in oxidative C(sp³)â€“H/C(sp)â€“H cross-coupling: an easy way toward the synthesis of furans and indolizines. Chemical Communications, 2015, 51, 8769-8772.	4.1	109
78	Dinuclear versus mononuclear pathways in zinc mediated nucleophilic addition: a combined experimental and DFT study. Dalton Transactions, 2015, 44, 11165-11171.	3.3	26
79	Silver Migration Facilitates Isocyanide-Alkyne [3 + 2] Cycloaddition Reactions: Combined Experimental and Theoretical Study. ACS Catalysis, 2015, 5, 6640-6647.	11.2	66
80	Copper-catalyzed aerobic oxidative coupling: From ketone and diamine to pyrazine. Science Advances, 2015, 1, e1500656.	10.3	24
81	Transitionâ€Metalâ€Free Formal Decarboxylative Coupling of Î±â€Oxocarboxylates with Î±â€Bromoketones under Neutral Conditions: A Simple Access to 1,3â€Diketones. Angewandte Chemie - International Edition, 2015, 54, 855-859.	13.8	34
82	Bimetallic zinc complex â€“ active species in coupling of terminal alkynes with aldehydes via nucleophilic addition/Oppenauer oxidation. Chemical Communications, 2015, 51, 576-579.	4.1	39
83	Revealing the halide effect on the kinetics of the aerobic oxidation of Cu(<scp>i</scp>) to Cu(<scp>ii</scp>). Chemical Communications, 2015, 51, 318-321.	4.1	21
84	Visibleâ€Lightâ€Mediated Decarboxylation/Oxidative Amidation of Î±â€Keto Acids with Amines under Mild Reaction Conditions Using O₂. Angewandte Chemie - International Edition, 2014, 53, 502-506.	13.8	375
85	Carbonâ€Centered Radical Addition to Oï£¾C of Amides or Esters as a Route to Cï£¿O Bond Formations. Chemistry - A European Journal, 2014, 20, 15605-15610.	3.3	56
86	Cu(II)â€“Cu(I) Synergistic Cooperation to Lead the Alkyne Câ€“H Activation. Journal of the American Chemical Society, 2014, 136, 16760-16763.	13.7	97
87	Reactivity for the Dielsâ€“Alder Reaction of Cumulenes: A Distortion-Interaction Analysis along the Reaction Pathway. Journal of Physical Chemistry A, 2014, 118, 2638-2645.	2.5	79
88	Transition-Metal-Assisted Radical/Radical Cross-Coupling: A New Strategy to the Oxidative C(sp³)â€“H/Nâ€“H Cross-Coupling. Organic Letters, 2014, 16, 3404-3407.	4.6	152
89	Revealing the solution structure of Pd(OAc) 2 with halide additives. Chinese Journal of Chemistry, 0, , .	4.9	5