Shi-Jun Li

List of Publications by Year
in descending order

74 papers	1,919 citations	257450 24 h-index	289244 40 g-index
75 all docs	75 docs citations	75 times ranked	1458 citing authors

#	Article	IF	Citations
1	Cooperative Multifunctional Organocatalysts for Ambient Conversion of Carbon Dioxide into Cyclic Carbonates. ACS Catalysis, 2018, 8, 9945-9957.	11.2	188
2	AIE Triggers the Circularly Polarized Luminescence of Atomically Precise Enantiomeric Copper(I) Alkynyl Clusters. Angewandte Chemie - International Edition, 2020, 59, 10052-10058.	13.8	165
3	4CzIPN-^tBu-Catalyzed Proton-Coupled Electron Transfer for Photosynthesis of Phosphorylated N-Heteroaromatics. Journal of the American Chemical Society, 2021, 143, 964-972.	13.7	135
4	Silver-catalyzed decarboxylative radical cascade cyclization toward benzimidazo[2,1-a]isoquinolin-6(5H)-ones. Chemical Communications, 2019, 55, 2861-2864.	4.1	114
5	Copper-Catalyzed Radical Cascade Cyclization To Access 3-Sulfonated Indenones with the AIE Phenomenon. Journal of Organic Chemistry, 2018, 83, 14419-14430.	3.2	74
6	Mn(III)â€Mediated Regioselective 6â€endoâ€trig Radical Cyclization of oâ€Vinylaryl Isocyanides to Access 2â€Functionalized Quinolines. Advanced Synthesis and Catalysis, 2020, 362, 688-694.	4.3	55
7	Carboranealkynylâ€Protected Gold Nanoclusters: Size Conversion and UV/Visâ€“NIR Optical Properties. Angewandte Chemie - International Edition, 2021, 60, 5959-5964.	13.8	52
8	Is Cu(<scp>iii</scp>) a necessary intermediate in Cu-mediated coupling reactions? A mechanistic point of view. Chemical Communications, 2020, 56, 6609-6619.	4.1	50
9	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.	4.1	48
10	Prediction of NHC-catalyzed chemoselective functionalizations of carbonyl compounds: a general mechanistic map. Chemical Science, 2020, 11, 7214-7225.	7.4	44
11	Boryl Radical Activation of Benzylic Câ€“OH Bond: Cross-Electrophile Coupling of Free Alcohols and CO₂ via Photoredox Catalysis. Journal of the American Chemical Society, 2022, 144, 8551-8559.	13.7	41
12	Ironâ€Catalyzed Radical Relay Enabling the Modular Synthesis of Fused Pyridines from Alkyneâ€Tethered Oximes and Alkenes. Angewandte Chemie - International Edition, 2020, 59, 23755-23762.	13.8	39
13	Insights into highly selective ring expansion of oxaziridines under Lewis base catalysis: a DFT study. Organic Chemistry Frontiers, 2019, 6, 679-687.	4.5	38
14	Multiple Functional Organocatalyst-Promoted Inert Câ€“C Activation: Mechanism and Origin of Selectivities. ACS Catalysis, 2021, 11, 3443-3454.	11.2	38
15	Hydrogenâ€Bondingâ€Promoted Cascade Rearrangement Involving the Enlargement of Two Rings: Efficient Access to Polycyclic Quinoline Derivatives. Angewandte Chemie - International Edition, 2020, 59, 21425-21430.	13.8	37
16	Catalytic Atroposelective Catellani Reaction Enables Construction of Axially Chiral Biaryl Monophosphine Oxides. CCS Chemistry, 2021, 3, 377-387.	7.8	37
17	AIE Triggers the Circularly Polarized Luminescence of Atomically Precise Enantiomeric Copper(I) Alkynyl Clusters. Angewandte Chemie, 2020, 132, 10138-10144.	2.0	34
18	Mechanism of Ir-catalyzed hydrogenation: A theoretical view. Coordination Chemistry Reviews, 2020, 412, 213251.	18.8	33

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19	A DFT kinetic study on 1,3-dipolar cycloaddition reactions in solution. Physical Chemistry Chemical Physics, 2016, 18, 30815-30823.	2.8	32
20	Atom Recombination of Difluorocarbene Enables 3-Fluorinated Oxindoles from 2-Aminoarylketones. CCS Chemistry, 2022, 4, 1671-1679.	7.8	32
21	Theoretical estimation of kinetic parameters for nucleophilic substitution reactions in solution: an application of a solution translational entropy model. Physical Chemistry Chemical Physics, 2016, 18, 6182-6190.	2.8	30
22	Elementalâ€Sulfurâ€Enabled Divergent Synthesis of Disulfides, Diselenides, and Polythiophenes from Î²â€CF₃â€1,3â€Enynes. Angewandte Chemie - International Edition, 2021, 60, 881-888.	13.8	30
23	Diradical Generation via Relayed Proton-Coupled Electron Transfer. Journal of the American Chemical Society, 2022, 144, 3137-3145.	13.7	29
24	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.	4.6	26
25	From Silica Sphere to Hollow Carbon Nitrideâ€Based Sphere: Rational Design of Sulfur Host with Both Chemisorption and Physical Confinement. Advanced Materials Interfaces, 2017, 4, 1601195.	3.7	25
26	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.	4.1	25
27	Pd^{IV} Species Mediation in Pd^{II}-Catalyzed Direct Alkylation of Arenes with Oxiranes: A DFT Study. Journal of Organic Chemistry, 2018, 83, 3142-3148.	3.2	24
28	Photo/Electrochromic Dual Responsive Behavior of a Cage-like Zr(IV)-Viologen Metalâ€“Organic Polyhedron (MOP). Inorganic Chemistry, 2022, 61, 2813-2823.	4.0	24
29	Regioselective Synthesis of Sulfonyl-Containing Benzyl Dithiocarbamates through Copper-Catalyzed Thiosulfonylation of Styrenes. Journal of Organic Chemistry, 2019, 84, 11135-11149.	3.2	21
30	A Theoretical Study of Ene Reactions in Solution: A Solutionâ€Phase Translational Entropy Model. ChemPhysChem, 2015, 16, 3711-3718.	2.1	20
31	Insights into Nâ€Heterocyclic Carbene (NHC)â€Catalyzed Asymmetric Addition of 2Hâ€Azirine with Aldehyde. Chemistry - an Asian Journal, 2019, 14, 2000-2007.	3.3	20
32	Insights into the chiral sulfide/selenide-catalyzed electrophilic carbothiolation of alkynes: mechanism and origin of axial chirality. Organic Chemistry Frontiers, 2021, 8, 1983-1990.	4.5	20
33	Deoxygenative Crossâ€Coupling of Aromatic Amides with Polyfluoroarenes. Angewandte Chemie - International Edition, 2022, 61, .	13.8	20
34	A DFT study on the competing mechanisms of PPh3-catalyzed [3+3] and [3+2] annulations between 5-acetoxypenta-2,3-dienoate and 1C,3O-bisnucleophiles. Journal of Molecular Catalysis A, 2015, 407, 137-146.	4.8	18
35	DFT Studies on the Dirhodium-Catalyzed [3 + 2] and [3 + 3] Cycloaddition Reactions of Enol Diazoacetates with Isoquinolinium Methylide: Mechanism, Selectivity, and Ligand Effect. Organometallics, 2018, 37, 1373-1380.	2.3	18
36	Organocatalytic insertion into Câ€“B bonds by in situ generated carbene: mechanism, role of the catalyst, and origin of stereoselectivity. Catalysis Science and Technology, 2022, 12, 947-953.	4.1	18

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37	Practical DMSO-promoted selective hydrolysisâ€“oxidation of lignocellulosic biomass to formic acid attributed to hydrogen bonds. Green Chemistry, 2021, 23, 7041-7052.	9.0	16
38	Carbene-enabled ether activation through the formation of oxonium: a theoretical view. Organic Chemistry Frontiers, 2022, 9, 1247-1253.	4.5	16
39	N-Heterocyclic carbene-catalyzed enantioselective hetero-[10â€‰+â€‰2] annulation. Communications Chemistry, 2020, 3, .	4.5	14
40	DFT studies on the distinct mechanisms of Câ€“H activation and oxidation reactions mediated by mononuclear- and binuclear-palladium. Dalton Transactions, 2018, 47, 6102-6111.	3.3	13
41	Insights into Lewis base-catalyzed chemoselective [3 + 2] and [3 + 4] annulation reactions of MBH carbonates. Organic Chemistry Frontiers, 2020, 7, 1828-1836.	4.5	13
42	Hydrogen radical-shuttle (HRS)-enabled photoredox synthesis of indanones via decarboxylative annulation. Nature Communications, 2021, 12, 5257.	12.8	12
43	Mechanistic investigation of zwitterionic MOF-catalyzed enyne annulation using UNLPF-14-MnIII as catalyst. Chinese Chemical Letters, 2022, 33, 4281-4286.	9.0	12
44	Theoretical studies on CuCl-catalyzed Câ€“H activation/Câ€“O coupling reactions: oxidant and catalyst effects. Organic and Biomolecular Chemistry, 2016, 14, 4426-4435.	2.8	11
45	Unravelling the Origins of Hydroboration Chemoselectivity Inversion Using an N,O-Chelated Ir(I) Complex: A Computational Study. Journal of Organic Chemistry, 2019, 84, 6709-6718.	3.2	10
46	Possible Mechanisms and Origin of Selectivities for Phosphineâ€Catalyzed [2+n] (n=3, 4) Annulations of Saturated Amines and Î²â€Acetoxy Allenoates. Asian Journal of Organic Chemistry, 2021, 10, 619-625.	2.7	10
47	How Solvents Control the Chemoselectivity in Rh-Catalyzed Defluorinated [4 + 1] Annulation. Organic Letters, 2021, 23, 1489-1494.	4.6	10
48	Understanding theZselectivity of the metal-free intermolecular aminoarylation of alkynes: a DFT study. Organic Chemistry Frontiers, 2019, 6, 125-133.	4.5	9
49	Ironâ€Catalyzed Radical Relay Enabling the Modular Synthesis of Fused Pyridines from Alkyneâ€Tethered Oximes and Alkenes. Angewandte Chemie, 2020, 132, 23963-23970.	2.0	9
50	Palladium-Catalyzed Asymmetric [3 + 2] Annulation of Vinylethylene Carbonates with Alkenes Installed on Cyclic N-Sulfonyl Imines: Highly Enantio- and Diastereoselective Construction of Chiral Tetrahydrofuran Scaffolds Bearing Three Vicinal and Quaternary Stereocenters. Journal of Organic Chemistry, 2022, 87, 5166-5177.	3.2	9
51	Origin and stabilization of axial chirality in the construction of naphthyl-C2-indoles: a DFT study. Organic Chemistry Frontiers, 2020, 7, 3166-3173.	4.5	8
52	Insights into isothiourea-catalyzed asymmetric [3 + 3] annulation of Î±,Î²-unsaturated aryl esters with 2-acylbenzazoles: mechanism, origin of stereoselectivity and switchable chemoselectivity. Catalysis Science and Technology, 2020, 10, 3664-3669.	4.1	8
53	A Computational Study on the 4â€Dimethylaminopyridine (DMAP)â€Catalyzed Regioselective [2+4] Cyclization of Allenic Ester with Cyclic Ketimine. ChemistrySelect, 2018, 3, 10553-10558.	1.5	7
54	Insight into Isothioureaâ€Catalyzed Enantioselective Addition of Saturated Esters to Iminium Ions. Chemistry - an Asian Journal, 2019, 14, 4322-4327.	3.3	6

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55	Carboranealkynylâ€Protected Gold Nanoclusters: Size Conversion and UV/Visâ€“NIR Optical Properties. Angewandte Chemie, 2021, 133, 6024-6029.	2.0	6
56	Semisynthesis of CRV431. Organic Letters, 2021, 23, 3421-3425.	4.6	6
57	Iminyl radical-triggered relay annulation for the construction of bridged aza-tetracycles bearing four contiguous stereogenic centers. Chemical Science, 2022, 13, 7283-7288.	7.4	6
58	The regioselectivity of the sulfonylation of tetrazoles: a theoretical view. Organic Chemistry Frontiers, 2022, 9, 4009-4015.	4.5	6
59	DFT studies on inclusion complexes of 1-phenyl-1-propanol enantiomers with modified cyclic decapeptides. Structural Chemistry, 2014, 25, 699-705.	2.0	5
60	Mechanism and Substituent Effects of Benzene Arylation via a Phenyl Cation Strategy: A Density Functional Theory Study. ChemCatChem, 2019, 11, 5068-5076.	3.7	5
61	Tunnelling assisted hydrogen elimination mechanisms of FeCl3/TEMPO. Chemical Communications, 2022, 58, 565-568.	4.1	5
62	Regioselectivity of Pd-catalyzed o-Carborane Arylation: A Theoretical View. Organic Chemistry Frontiers, 0, , .	4.5	5
63	Design and synthesis of stable four-coordinated benzotriazole-borane with tunable fluorescence emission. Chemical Science, 2022, 13, 5982-5987.	7.4	5
64	Mechanistic Study of Cu-Catalyzed Addition Reaction of Isocyanates. Chinese Journal of Organic Chemistry, 2021, 41, 4347.	1.3	4
65	A New Intermetallic NiSn₅ Phase: Induced Synthesis, Crystal Structure Resolution, and Investigation of Its Mechanism. Journal of Physical Chemistry Letters, 2019, 10, 2561-2566.	4.6	3
66	Elementalâ€Sulfurâ€Enabled Divergent Synthesis of Disulfides, Diselenides, and Polythiophenes from Î²â€CF 3 â€1,3â€Enynes. Angewandte Chemie, 2021, 133, 894-901.	2.0	3
67	How to inverse the chemoselectivity of nucleophilic addition by using a Lewis acid/BrÃ¸nsted base pair catalyst: A theoretical view. Molecular Catalysis, 2021, 499, 111318.	2.0	3
68	Hydrogenâ€Bondingâ€Promoted Cascade Rearrangement Involving the Enlargement of Two Rings: Efficient Access to Polycyclic Quinoline Derivatives. Angewandte Chemie, 2020, 132, 21609-21614.	2.0	2
69	Is the reaction sequence in phosphine-catalyzed [8+2] cycloaddition controlled by electrophilicity?. Chemical Communications, 2021, 57, 761-764.	4.1	2
70	Deoxygenative Crossâ€Coupling of Aromatic Amides with Polyfluoroarenes. Angewandte Chemie, 0, , .	2.0	2
71	Syntheses, Structures of Two Coordination Polymers Based on Bipyridyl and Carboxyl Groups. Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry, 2012, 42, 1078-1082.	0.6	1
72	Origin of stereoselectivity in an isothiourea catalyzed Michael addition reaction of aryl ester with vinyl disulfone. New Journal of Chemistry, 2020, 44, 17906-17911.	2.8	1

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73	Origin of diastereoselectivity and catalytic efficiency on Isothiourea-mediated cyclization of carboxylic acid with alkenyl ketone. Computational and Theoretical Chemistry, 2020, 1190, 113004.	2.5	1
74	Theoretical study on mechanism of cycloaddition reaction between o-alkynylbenzaldoximes and hexynol catalyzed by silver(I). Molecular Catalysis, 2022, 522, 112227.	2.0	0