

# Shi-Jun Li

## List of Publications by Year in descending order

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74  
papers

1,919  
citations

257450

24  
h-index

289244

40  
g-index

75  
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75  
docs citations

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times ranked

1458  
citing authors

#	ARTICLE	IF	CITATIONS
1	Atom Recombination of Difluorocarbene Enables 3-Fluorinated Oxindoles from 2-Aminoarylketones. <i>CCS Chemistry</i> , 2022, 4, 1671-1679.	7.8	32
2	Tunnelling assisted hydrogen elimination mechanisms of FeCl <sub>3</sub> /TEMPO. <i>Chemical Communications</i> , 2022, 58, 565-568.	4.1	5
3	Mechanistic investigation of zwitterionic MOF-catalyzed enyne annulation using UNLPF-14-MnIII as catalyst. <i>Chinese Chemical Letters</i> , 2022, 33, 4281-4286.	9.0	12
4	Carbene-enabled ether activation through the formation of oxonium: a theoretical view. <i>Organic Chemistry Frontiers</i> , 2022, 9, 1247-1253.	4.5	16
5	Deoxygenative Cross-Coupling of Aromatic Amides with Polyfluoroarenes. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	20
6	Organocatalytic insertion into C=C bonds by <i>in situ</i> generated carbene: mechanism, role of the catalyst, and origin of stereoselectivity. <i>Catalysis Science and Technology</i> , 2022, 12, 947-953.	4.1	18
7	Photo/Electrochromic Dual Responsive Behavior of a Cage-like Zr(IV)-Viologen Metal-Organic Polyhedron (MOP). <i>Inorganic Chemistry</i> , 2022, 61, 2813-2823.	4.0	24
8	Diradical Generation via Relayed Proton-Coupled Electron Transfer. <i>Journal of the American Chemical Society</i> , 2022, 144, 3137-3145.	13.7	29
9	Theoretical study on mechanism of cycloaddition reaction between <i>o</i> -alkynylbenzaldoximes and hexynol catalyzed by silver(I). <i>Molecular Catalysis</i> , 2022, 522, 112227.	2.0	0
10	Boryl Radical Activation of Benzylic C-OH Bond: Cross-Electrophile Coupling of Free Alcohols and CO <sub>2</sub> via Photoredox Catalysis. <i>Journal of the American Chemical Society</i> , 2022, 144, 8551-8559.	13.7	41
11	Palladium-Catalyzed Asymmetric [3 + 2] Annulation of Vinyl-ethylene Carbonates with Alkenes Installed on Cyclic N-Sulfonyl Imines: Highly Enantio- and Diastereoselective Construction of Chiral Tetrahydrofuran Scaffolds Bearing Three Vicinal and Quaternary Stereocenters. <i>Journal of Organic Chemistry</i> , 2022, 87, 5166-5177.	3.2	9
12	Design and synthesis of stable four-coordinated benzotriazole-borane with tunable fluorescence emission. <i>Chemical Science</i> , 2022, 13, 5982-5987.	7.4	5
13	Iminyl radical-triggered relay annulation for the construction of bridged aza-tetracycles bearing four contiguous stereogenic centers. <i>Chemical Science</i> , 2022, 13, 7283-7288.	7.4	6
14	The regioselectivity of the sulfonylation of tetrazoles: a theoretical view. <i>Organic Chemistry Frontiers</i> , 2022, 9, 4009-4015.	4.5	6
15	Elemental Sulfur-Enabled Divergent Synthesis of Disulfides, Diselenides, and Polythiophenes from $\text{I}_2\text{CF}_3$ and Enynes. <i>Angewandte Chemie</i> , 2021, 133, 894-901.	2.0	3
16	Elemental Sulfur-Enabled Divergent Synthesis of Disulfides, Diselenides, and Polythiophenes from $\text{I}_2\text{CF}_3$ and Enynes. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 881-888.	13.8	30
17	How to inverse the chemoselectivity of nucleophilic addition by using a Lewis acid/Brønsted base pair catalyst: A theoretical view. <i>Molecular Catalysis</i> , 2021, 499, 111318.	2.0	3
18	Possible Mechanisms and Origin of Selectivities for Phosphine-Catalyzed [2+n] (n=3, 4) Annulations of Saturated Amines and Acetoxy Allenates. <i>Asian Journal of Organic Chemistry</i> , 2021, 10, 619-625.	2.7	10

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19	Carboranealkynyl-Protected Gold Nanoclusters: Size Conversion and UV/Vis-NIR Optical Properties. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 5959-5964.	13.8	52
20	Is the reaction sequence in phosphine-catalyzed [8+2] cycloaddition controlled by electrophilicity?. <i>Chemical Communications</i> , 2021, 57, 761-764.	4.1	2
21	Carboranealkynyl-Protected Gold Nanoclusters: Size Conversion and UV/Vis-NIR Optical Properties. <i>Angewandte Chemie</i> , 2021, 133, 6024-6029.	2.0	6
22	Insights into the chiral sulfide/selenide-catalyzed electrophilic carbothiolation of alkynes: mechanism and origin of axial chirality. <i>Organic Chemistry Frontiers</i> , 2021, 8, 1983-1990.	4.5	20
23	Catalytic Atroposelective Catellani Reaction Enables Construction of Axially Chiral Biaryl Monophosphine Oxides. <i>CCS Chemistry</i> , 2021, 3, 377-387.	7.8	37
24	How Solvents Control the Chemoselectivity in Rh-Catalyzed Defluorinated [4 + 1] Annulation. <i>Organic Letters</i> , 2021, 23, 1489-1494.	4.6	10
25	Multiple Functional Organocatalyst-Promoted Inert C-C Activation: Mechanism and Origin of Selectivities. <i>ACS Catalysis</i> , 2021, 11, 3443-3454.	11.2	38
26	Theoretical Model for N-Heterocyclic Carbene-Catalyzed Desymmetrizing [4 + 1] and [4 + 2] Annulations of an Enal and Aryldialdehyde with 1,3-Cyclopentenedione. <i>Organic Letters</i> , 2021, 23, 2421-2425.	4.6	26
27	Semisynthesis of CRV431. <i>Organic Letters</i> , 2021, 23, 3421-3425.	4.6	6
28	Hydrogen radical-shuttle (HRS)-enabled photoredox synthesis of indanones via decarboxylative annulation. <i>Nature Communications</i> , 2021, 12, 5257.	12.8	12
29	Practical DMSO-promoted selective hydrolysis-oxidation of lignocellulosic biomass to formic acid attributed to hydrogen bonds. <i>Green Chemistry</i> , 2021, 23, 7041-7052.	9.0	16
30	4CzIPN-t-Bu-Catalyzed Proton-Coupled Electron Transfer for Photosynthesis of Phosphorylated N-Heteroaromatics. <i>Journal of the American Chemical Society</i> , 2021, 143, 964-972.	13.7	135
31	Mechanistic Study of Cu-Catalyzed Addition Reaction of Isocyanates. <i>Chinese Journal of Organic Chemistry</i> , 2021, 41, 4347.	1.3	4
32	AIE Triggers the Circularly Polarized Luminescence of Atomically Precise Enantiomeric Copper(I) Alkynyl Clusters. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 10052-10058.	13.8	165
33	AIE Triggers the Circularly Polarized Luminescence of Atomically Precise Enantiomeric Copper(I) Alkynyl Clusters. <i>Angewandte Chemie</i> , 2020, 132, 10138-10144.	2.0	34
34	Mn(III)-Mediated Regioselective 6-endo-trig Radical Cyclization of Vinylaryl Isocyanides to Access 2-Functionalized Quinolines. <i>Advanced Synthesis and Catalysis</i> , 2020, 362, 688-694.	4.3	55
35	N-Heterocyclic carbene-catalyzed enantioselective hetero-[10+2] annulation. <i>Communications Chemistry</i> , 2020, 3, .	4.5	14
36	Hydrogen-Bonding-Promoted Cascade Rearrangement Involving the Enlargement of Two Rings: Efficient Access to Polycyclic Quinoline Derivatives. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 21425-21430.	13.8	37

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37	Hydrogen-Bonding-Promoted Cascade Rearrangement Involving the Enlargement of Two Rings: Efficient Access to Polycyclic Quinoline Derivatives. <i>Angewandte Chemie</i> , 2020, 132, 21609-21614.	2.0	2
38	Iron-Catalyzed Radical Relay Enabling the Modular Synthesis of Fused Pyridines from Alkyne-Tethered Oximes and Alkenes. <i>Angewandte Chemie</i> , 2020, 132, 23963-23970.	2.0	9
39	Origin and stabilization of axial chirality in the construction of naphthyl-C2-indoles: a DFT study. <i>Organic Chemistry Frontiers</i> , 2020, 7, 3166-3173.	4.5	8
40	Origin of stereoselectivity in an isothiourea catalyzed Michael addition reaction of aryl ester with vinyl disulfone. <i>New Journal of Chemistry</i> , 2020, 44, 17906-17911.	2.8	1
41	Iron-Catalyzed Radical Relay Enabling the Modular Synthesis of Fused Pyridines from Alkyne-Tethered Oximes and Alkenes. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 23755-23762.	13.8	39
42	Origin of diastereoselectivity and catalytic efficiency on Isothiourea-mediated cyclization of carboxylic acid with alkenyl ketone. <i>Computational and Theoretical Chemistry</i> , 2020, 1190, 113004.	2.5	1
43	Insights into isothiourea-catalyzed asymmetric [3 + 3] annulation of $\beta,\beta$ -unsaturated aryl esters with 2-acylbenzazoles: mechanism, origin of stereoselectivity and switchable chemoselectivity. <i>Catalysis Science and Technology</i> , 2020, 10, 3664-3669.	4.1	8
44	Is Cu a necessary intermediate in Cu-mediated coupling reactions? A mechanistic point of view. <i>Chemical Communications</i> , 2020, 56, 6609-6619.	4.1	50
45	Prediction of NHC-catalyzed chemoselective functionalizations of carbonyl compounds: a general mechanistic map. <i>Chemical Science</i> , 2020, 11, 7214-7225.	7.4	44
46	Insights into Lewis base-catalyzed chemoselective [3 + 2] and [3 + 4] annulation reactions of MBH carbonates. <i>Organic Chemistry Frontiers</i> , 2020, 7, 1828-1836.	4.5	13
47	With metal or not? a computationally predicted rule for a dirhodium catalyst in [3+3] cycloadditions of triazole with thiirane. <i>Chemical Communications</i> , 2020, 56, 4732-4735.	4.1	25
48	Mechanism of Ir-catalyzed hydrogenation: A theoretical view. <i>Coordination Chemistry Reviews</i> , 2020, 412, 213251.	18.8	33
49	Mechanism and Substituent Effects of Benzene Arylation via a Phenyl Cation Strategy: A Density Functional Theory Study. <i>ChemCatChem</i> , 2019, 11, 5068-5076.	3.7	5
50	Regioselective Synthesis of Sulfonyl-Containing Benzyl Dithiocarbamates through Copper-Catalyzed Thiosulfonylation of Styrenes. <i>Journal of Organic Chemistry</i> , 2019, 84, 11135-11149.	3.2	21
51	Insight into Isothiourea-Catalyzed Enantioselective Addition of Saturated Esters to Iminium Ions. <i>Chemistry - an Asian Journal</i> , 2019, 14, 4322-4327.	3.3	6
52	Understanding the <i>Z</i> -selectivity of the metal-free intermolecular aminoarylation of alkynes: a DFT study. <i>Organic Chemistry Frontiers</i> , 2019, 6, 125-133.	4.5	9
53	Insights into highly selective ring expansion of oxaziridines under Lewis base catalysis: a DFT study. <i>Organic Chemistry Frontiers</i> , 2019, 6, 679-687.	4.5	38
54	Unravelling the Origins of Hydroboration Chemoselectivity Inversion Using an N,O-Chelated Ir(I) Complex: A Computational Study. <i>Journal of Organic Chemistry</i> , 2019, 84, 6709-6718.	3.2	10

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55	A New Intermetallic NiSn <sub>5</sub> Phase: Induced Synthesis, Crystal Structure Resolution, and Investigation of Its Mechanism. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2561-2566.	4.6	3
56	Insights into NHC-catalyzed oxidative $\alpha$ -C(sp <sup>3</sup> ) $\alpha$ -H activation of aliphatic aldehydes and cascade [2 + 3] cycloaddition with azomethine imines. <i>Catalysis Science and Technology</i> , 2019, 9, 2514-2522.	4.1	48
57	Insights into N-Heterocyclic Carbene (NHC)-Catalyzed Asymmetric Addition of 2H-Azirine with Aldehyde. <i>Chemistry - an Asian Journal</i> , 2019, 14, 2000-2007.	3.3	20
58	Silver-catalyzed decarboxylative radical cascade cyclization toward benzimidazo[2,1- <i>a</i> ]isoquinolin-6(5 <i>H</i> )-ones. <i>Chemical Communications</i> , 2019, 55, 2861-2864.	4.1	114
59	Pd <sup>IV</sup> Species Mediation in Pd <sup>II</sup> -Catalyzed Direct Alkylation of Arenes with Oxiranes: A DFT Study. <i>Journal of Organic Chemistry</i> , 2018, 83, 3142-3148.	3.2	24
60	DFT Studies on the Dirhodium-Catalyzed [3 + 2] and [3 + 3] Cycloaddition Reactions of Enol Diazoacetates with Isoquinolinium Methylide: Mechanism, Selectivity, and Ligand Effect. <i>Organometallics</i> , 2018, 37, 1373-1380.	2.3	18
61	DFT studies on the distinct mechanisms of C $\alpha$ -H activation and oxidation reactions mediated by mononuclear- and binuclear-palladium. <i>Dalton Transactions</i> , 2018, 47, 6102-6111.	3.3	13
62	A Computational Study on the 4 $\alpha$ -Dimethylaminopyridine (DMAP)-Catalyzed Regioselective [2+4] Cyclization of Allenic Ester with Cyclic Ketimine. <i>ChemistrySelect</i> , 2018, 3, 10553-10558.	1.5	7
63	Copper-Catalyzed Radical Cascade Cyclization To Access 3-Sulfonated Indenones with the AIE Phenomenon. <i>Journal of Organic Chemistry</i> , 2018, 83, 14419-14430.	3.2	74
64	Cooperative Multifunctional Organocatalysts for Ambient Conversion of Carbon Dioxide into Cyclic Carbonates. <i>ACS Catalysis</i> , 2018, 8, 9945-9957.	11.2	188
65	From Silica Sphere to Hollow Carbon Nitride-Based Sphere: Rational Design of Sulfur Host with Both Chemisorption and Physical Confinement. <i>Advanced Materials Interfaces</i> , 2017, 4, 1601195.	3.7	25
66	Theoretical studies on CuCl-catalyzed C $\alpha$ -H activation/C $\alpha$ -O coupling reactions: oxidant and catalyst effects. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 4426-4435.	2.8	11
67	A DFT kinetic study on 1,3-dipolar cycloaddition reactions in solution. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 30815-30823.	2.8	32
68	Theoretical estimation of kinetic parameters for nucleophilic substitution reactions in solution: an application of a solution translational entropy model. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 6182-6190.	2.8	30
69	A Theoretical Study of Ene Reactions in Solution: A Solution-Phase Translational Entropy Model. <i>ChemPhysChem</i> , 2015, 16, 3711-3718.	2.1	20
70	A DFT study on the competing mechanisms of PPh <sub>3</sub> -catalyzed [3+3] and [3+2] annulations between 5-acetoxypenta-2,3-dienoate and 1C,3O-bisnucleophiles. <i>Journal of Molecular Catalysis A</i> , 2015, 407, 137-146.	4.8	18
71	DFT studies on inclusion complexes of 1-phenyl-1-propanol enantiomers with modified cyclic decapeptides. <i>Structural Chemistry</i> , 2014, 25, 699-705.	2.0	5
72	Syntheses, Structures of Two Coordination Polymers Based on Bipyridyl and Carboxyl Groups. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , 2012, 42, 1078-1082.	0.6	1

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73	Deoxygenative Cross-Coupling of Aromatic Amides with Polyfluoroarenes. <i>Angewandte Chemie</i> , , .	2.0	2
74	Regioselectivity of Pd-catalyzed o-Carborane Arylation: A Theoretical View. <i>Organic Chemistry Frontiers</i> , , .	4.5	5