Jin-Shuai Song

List of Publications by Year
in descending order

76 papers	3,955 citations	94433 37 h-index	123424 61 g-index
83 all docs	83 docs citations	83 times ranked	2888 citing authors

#	Article	IF	Citations
1	Electrochemical Câ€”H/Nâ€”H Functionalization for the Synthesis of Highly Functionalized (Aza)indoles. Angewandte Chemie - International Edition, 2016, 55, 9168-9172.	13.8	215
2	Electrochemical Difluoromethylarylation of Alkynes. Journal of the American Chemical Society, 2018, 140, 2460-2464.	13.7	215
3	Amidinyl Radical Formation through Anodic Nâ€”H Bond Cleavage and Its Application in Aromatic Câ€”H Bond Functionalization. Angewandte Chemie - International Edition, 2017, 56, 587-590.	13.8	179
4	TEMPO-Catalyzed Electrochemical Câ€“H Thiolation: Synthesis of Benzothiazoles and Thiazolopyridines from Thioamides. ACS Catalysis, 2017, 7, 2730-2734.	11.2	178
5	Electrophotocatalytic Decarboxylative Câ€”H Functionalization of Heteroarenes. Angewandte Chemie - International Edition, 2020, 59, 10626-10632.	13.8	161
6	The Mechanism of Homogeneous CO₂ Reduction by Ni(cyclam): Product Selectivity, Concerted Protonâ€“Electron Transfer and Câ€“O Bond Cleavage. Inorganic Chemistry, 2014, 53, 7500-7507.	4.0	145
7	Reagentâ€Free Câ€”H/Nâ€”H Crossâ€Coupling: Regioselective Synthesis of Nâ€Heteroaromatics from Biaryl Aldehydes and NH₃. Angewandte Chemie - International Edition, 2017, 56, 12732-12735.	13.8	132
8	Electrochemically Enabled Carbohydroxylation of Alkenes with H₂O and Organotrifluoroborates. Journal of the American Chemical Society, 2018, 140, 16387-16391.	13.7	127
9	Electrochemical Synthesis of Polycyclic N-Heteroaromatics through Cascade Radical Cyclization of Diynes. ACS Catalysis, 2017, 7, 5810-5813.	11.2	124
10	Siteâ€Selective Electrochemical Benzylic Câ€”H Amination. Angewandte Chemie - International Edition, 2021, 60, 2943-2947.	13.8	123
11	The Inverted Bond in [1.1.1]Propellane is a Chargeâ€Shift Bond. Angewandte Chemie - International Edition, 2009, 48, 1407-1410.	13.8	120
12	Cathode Material Determines Product Selectivity for Electrochemical Câ€”H Functionalization of Biaryl Ketoximes. Angewandte Chemie - International Edition, 2018, 57, 15153-15156.	13.8	112
13	Scalable Rhodium(III)â€Catalyzed Aryl Câ€”H Phosphorylation Enabled by Anodic Oxidation Induced Reductive Elimination. Angewandte Chemie - International Edition, 2019, 58, 16770-16774.	13.8	111
14	Bio-inspired mechanistic insights into CO2 reduction. Current Opinion in Chemical Biology, 2015, 25, 103-109.	6.1	88
15	Electronic Structure of a Formal Iron(0) Porphyrin Complex Relevant to CO₂ Reduction. Inorganic Chemistry, 2017, 56, 4745-4750.	4.0	85
16	Siteâ€Selective Electrochemical Benzylic Câ€”H Amination. Angewandte Chemie, 2021, 133, 2979-2983.	2.0	81
17	Metal-free atom transfer radical polymerization with ppm catalyst loading under sunlight. Nature Communications, 2021, 12, 429.	12.8	72
18	Multiple Low-Lying States for Compound I of P450_{cam}and Chloroperoxidase Revealed from Multireference Ab Initio QM/MM Calculations. Journal of Chemical Theory and Computation, 2010, 6, 940-953.	5.3	66

#	Article	IF	Citations
19	Radical Fluorosulfonylation: Accessing Alkenyl Sulfonyl Fluorides from Alkenes. Angewandte Chemie - International Edition, 2021, 60, 3956-3960.	13.8	66
20	XMVB 2.0: A new version of Xiamen valence bond program. International Journal of Quantum Chemistry, 2015, 115, 731-737.	2.0	65
21	De Novo Synthesis of Highly Functionalized Benzimidazolones and Benzoxazolones through an Electrochemical Dehydrogenative Cyclization Cascade. Angewandte Chemie - International Edition, 2019, 58, 9017-9021.	13.8	65
22	Electrochemical Synthesis of (Aza)indolines via Dehydrogenative [3+2] Annulation: Application to Total Synthesis of (Â±)â€Hinckdentine A. Chinese Journal of Chemistry, 2018, 36, 909-915.	4.9	63
23	Electrochemical Câˆ'H/Nâˆ'H Functionalization for the Synthesis of Highly Functionalized (Aza)indoles. Angewandte Chemie, 2016, 128, 9314-9318.	2.0	56
24	Easy access to medium-sized lactones through metal carbene migratory insertion enabled 1,4-palladium shift. Nature Communications, 2020, 11, 461.	12.8	55
25	Aminofluorination: transition-metal-free Nâ€“F bond insertion into diazocarbonyl compounds. Chemical Science, 2016, 7, 1786-1790.	7.4	53
26	Copperâ€Catalyzed Intramolecular Oxidative Amination of Unactivated Internal Alkenes. Chemistry - A European Journal, 2016, 22, 4379-4383.	3.3	52
27	An efficient algorithm for energy gradients and orbital optimization in valence bond theory. Journal of Computational Chemistry, 2009, 30, 399-406.	3.3	50
28	Optical Resolution of the Water-Soluble Ti₄(embonate)₆ Cages for Enantioselective Recognition of Chiral Drugs. Chemistry of Materials, 2018, 30, 7769-7775.	6.7	49
29	Electrochemical Difluoromethylation of Electronâ€Deficient Alkenes. ChemSusChem, 2019, 12, 3060-3063.	6.8	48
30	Catalystâ€•and Reagentâ€Free Formal Azaâ€Wacker Cyclizations Enabled by Continuousâ€Flow Electrochemistry. Angewandte Chemie - International Edition, 2021, 60, 11237-11241.	13.8	47
31	Valence bond modelling and density functional theory calculations of reactivity and mechanism of cytochrome P450 enzymes: thioether sulfoxidation. Faraday Discussions, 0, 145, 49-70.	3.2	45
32	Tailored cobalt-salen complexes enable electrocatalytic intramolecular allylic Câ€“H functionalizations. Nature Communications, 2021, 12, 3745.	12.8	44
33	Valence Bond Perturbation Theory. A Valence Bond Method That Incorporates Perturbation Theory. Journal of Physical Chemistry A, 2009, 113, 11560-11569.	2.5	43
34	Organoelectrocatalysis Enables Direct Cyclopropanation of Methylene Compounds. Journal of the American Chemical Society, 2022, 144, 2343-2350.	13.7	43
35	Amidinyl Radical Formation through Anodic Nâˆ'H Bond Cleavage and Its Application in Aromatic Câˆ'H Bond Functionalization. Angewandte Chemie, 2017, 129, 602-605.	2.0	42
36	Computational advances aiding mechanistic understanding of silver-catalyzed carbene/nitrene/silylene transfer reactions. Coordination Chemistry Reviews, 2019, 382, 69-84.	18.8	42

#	Article	IF	Citations
37	Electrochemical synthesis of 7-membered carbocycles through cascade 5-exo-trig/7-endo-trig radical cyclization. Organic Chemistry Frontiers, 2018, 5, 3129-3132.	4.5	40
38	Electrocatalytic Allylic Câˆ'H Alkylation Enabled by a Dualâ€Function Cobalt Catalyst**. Angewandte Chemie - International Edition, 2022, 61, .	13.8	40
39	Electrochemical Câ€"H phosphorylation of arenes in continuous flow suitable for late-stage functionalization. Nature Communications, 2021, 12, 6629.	12.8	38
40	Synthesis of Acridinium Photocatalysts via Site-Selective Câ€"H Alkylation. CCS Chemistry, 2021, 3, 317-325.	7.8	37
41	Theory Demonstrated a â€œCoupledâ€•Mechanism for O₂ Activation and Substrate Hydroxylation by Binuclear Copper Monooxygenases. Journal of the American Chemical Society, 2019, 141, 19776-19789.	13.7	36
42	Scalable Rhodium(III)â€Catalyzed Aryl Câˆ'H Phosphorylation Enabled by Anodic Oxidation Induced Reductive Elimination. Angewandte Chemie, 2019, 131, 16926-16930.	2.0	35
43	Reagentâ€Free Câˆ'H/Nâˆ'H Crossâ€Coupling: Regioselective Synthesis of Nâ€Heteroaromatics from Biaryl Aldehydes and NH₃. Angewandte Chemie, 2017, 129, 12906-12909.	2.0	34
44	Cathode Material Determines Product Selectivity for Electrochemical Câˆ'H Functionalization of Biaryl Ketoximes. Angewandte Chemie, 2018, 130, 15373-15376.	2.0	32
45	Fenton-Derived OH Radicals Enable the MPnS Enzyme to Convert 2-Hydroxyethylphosphonate to Methylphosphonate: Insights from Ab Initio QM/MM MD Simulations. Journal of the American Chemical Society, 2019, 141, 9284-9291.	13.7	32
46	Electrophotocatalytic Decarboxylative Câˆ'H Functionalization of Heteroarenes. Angewandte Chemie, 2020, 132, 10713-10719.	2.0	30
47	Diradical Generation via Relayed Proton-Coupled Electron Transfer. Journal of the American Chemical Society, 2022, 144, 3137-3145.	13.7	29
48	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.	4.5	25
49	Electrochemical aromatic Câ€"H hydroxylation in continuous flow. Nature Communications, 2022, 13, .	12.8	23
50	Electrocatalytic Dehydrogenative Cyclization of 2-Vinylanilides for the Synthesis of Indoles. Journal of Organic Chemistry, 2021, 86, 16001-16007.	3.2	22
51	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
52	Radical Fluorosulfonylation: Accessing Alkenyl Sulfonyl Fluorides from Alkenes. Angewandte Chemie, 2021, 133, 4002-4006.	2.0	18
53	BrÃ¸nsted base-catalyzed annulation of allyl ketones and alkynyl 1,2-diketones. Chemical Communications, 2018, 54, 4266-4269.	4.1	14
54	De Novo Synthesis of Highly Functionalized Benzimidazolones and Benzoxazolones through an Electrochemical Dehydrogenative Cyclization Cascade. Angewandte Chemie, 2019, 131, 9115-9119.	2.0	14

#	Article	IF	Citations
55	HOTf-Catalyzed Alkyl-Heck-type Reaction. IScience, 2018, 3, 255-263.	4.1	13
56	An efficient algorithm for complete active space valence bond selfâ€consistent field calculation. Journal of Computational Chemistry, 2013, 34, 38-48.	3.3	12
57	A diastereoselective approach to axially chiral biaryls via electrochemically enabled cyclization cascade. Beilstein Journal of Organic Chemistry, 2019, 15, 795-800.	2.2	12
58	Mechanistic investigation of zwitterionic MOF-catalyzed enyne annulation using UNLPF-14-MnIII as catalyst. Chinese Chemical Letters, 2022, 33, 4281-4286.	9.0	12
59	Mechanistic Insights into the Directing Effect of Thr303 in Ethanol Oxidation by Cytochrome P450 2E1. ACS Catalysis, 2019, 9, 4892-4901.	11.2	11
60	Electrocatalytic Allylic Cå^'H Alkylation Enabled by a Dualâ€Function Cobalt Catalyst**. Angewandte Chemie, 2022, 134, .	2.0	10
61	Bâ€Heterocyclic Carbene Arising from Charge Shift: A Computational Verification. Chemistry - A European Journal, 2018, 24, 10216-10223.	3.3	8
62	Synthesis, crystal structure and MMCT of new cyanide-bridged complexes cis-M^{II}(dppm)₂(CN)₂(Fe^{III}X₃)₂ (M = Ru, Os). RSC Advances, 2015, 5, 3399-3407.	3.6	7
63	A theoretical study on the mechanism of hydrogenation of carboxylic acids catalyzed by the Saito catalyst. Dalton Transactions, 2018, 47, 2460-2469.	3.3	7
64	A VALENCE BOND APPROACH BASED ON LEWIS STRUCTURES. Journal of Theoretical and Computational Chemistry, 2008, 07, 655-668.	1.8	6
65	Bonding and Dielsâ€"Alder reactions of substituted 2-borabicyclo(1.1.0)but-1(3)-enes: a theoretical study. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	6
66	Mechanistic insights into the crucial roles of Glu76 residue in nickel-dependent quercetin 2,4-dioxygenase for quercetin oxidative degradation. Journal of Catalysis, 2020, 387, 73-83.	6.2	3
67	N-Body Reduced Density Matrix-Based Valence Bond Theory and Its Applications in Diabatic Electronic-Structure Computations. Accounts of Chemical Research, 2021, 54, 3895-3905.	15.6	3
68	Frontispiece: Electrochemical Cå^'H/Nå^'H Functionalization for the Synthesis of Highly Functionalized (Aza)indoles. Angewandte Chemie - International Edition, 2016, 55, .	13.8	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	Catalystâ€•and Reagentâ€Free Formal Azaâ€Wacker Cyclizations Enabled by Continuousâ€Flow Electrochemistry. Angewandte Chemie, 2021, 133, 11337-11341.	2.0	2
71	Solvent-dependent tautomeric equilibrium between fluorescent colorimetric probes with dual mitochondrial/liposome targetability. Dyes and Pigments, 2021, 191, 109377.	3.7	2
72	Side-On versus End-On Binding Modes between Metal Cations and (NHC)AlAl(NHC). Organometallics, 2020, 39, 3240-3249.	2.3	1

#	Article	IF	Citations
73	Frontispiz: Electrochemical Câ^'H/Nâ^'H Functionalization for the Synthesis of Highly Functionalized (Aza)indoles. Angewandte Chemie, 2016, 128, .	2.0	0
74	Beryllium and boron decoration form planar tetracoordinate carbon strips at the edge of BCN nanoribbons result in energy gap opposite variation and third-order nonlinear optical response improvement. Chemical Physics Letters, 2017, 685, 432-437.	2.6	0
75	Innentitelbild: De Novo Synthesis of Highly Functionalized Benzimidazolones and Benzoxazolones through an Electrochemical Dehydrogenative Cyclization Cascade (Angew. Chem. 27/2019). Angewandte Chemie, 2019, 131, 9042-9042.	2.0	0
76	InnenrÃ¼cktitelbild: Scalable Rhodium(III)â€Catalyzed Aryl Câ^'H Phosphorylation Enabled by Anodic Oxidation Induced Reductive Elimination (Angew. Chem. 47/2019). Angewandte Chemie, 2019, 131, 17239-17239.	2.0	0