

Siwei Bi

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

88

papers

910

citations

17

h-index

24

g-index

89

ext. papers

1,050

ext. citations

4

avg, IF

4.59

L-index

#	Paper	IF	Citations
88	Decarbonylative Issues Involved in Ru(II)-Catalyzed [6+2 π] Annulation Reaction of Hydroxychromone with Alkyne: A DFT Study. <i>European Journal of Organic Chemistry</i> , 2021 , 2021, 266-273 ^{3.2}		2
87	Electronic Spin Moment As a Catalytic Descriptor for Fe Single-Atom Catalysts Supported on CN. <i>Journal of the American Chemical Society</i> , 2021 , 143, 4405-4413	16.4	40
86	Mechanism and selectivity on Ir(III)/Rh(III)-catalyzed coupling of terminal alkenes and dioxazolones: A DFT study. <i>Molecular Catalysis</i> , 2021 , 510, 111679	3.3	1
85	Theoretical evaluation of the carbene-based site-selectivity in gold(III)-catalyzed annulations of alkynes with anthranils. <i>Chemical Communications</i> , 2021 , 57, 1494-1497	5.8	2
84	Design of an efficient photocatalyst: a type II heterojunction for enhanced hydrogen production driven by visible light. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 11893-11899	3.6	4
83	How size, edge shape, functional groups and embeddedness influence the electronic structure and partial optical properties of graphene nanoribbons. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 20695-20701 ^{3.6}		20701 ²
82	Double-Regiodetermining-Stages Mechanistic Model Explaining the Regioselectivity of Pd-Catalyzed Hydroaminocarbonylation of Alkenes with Carbon Monoxide and Ammonium Chloride. <i>Journal of Organic Chemistry</i> , 2021 , 86, 12988-13000	4.2	1
81	Computational Study on the Mechanisms and Origins of Selectivity in Hydroarylation of 1,3-Diyne Alcohol Catalyzed by Di- and Mononuclear Manganese Complexes. <i>Organometallics</i> , 2021 , 40, 3124-3135 ^{3.8}		1
80	Substituent-dependent generation of tricyclic frameworks by the rhodium-catalyzed cycloisomerization of homopropargyl allene-alkynes: a theoretical study. <i>Dalton Transactions</i> , 2020 , 49, 7406-7419	4.3	1
79	Mechanism and Origin of Ligand-Controlled Chemo- and Regioselectivities in Palladium-Catalyzed Methoxycarbonylation of Alkynes. <i>Journal of Organic Chemistry</i> , 2020 , 85, 7136-7151	4.2	10
78	Density Functional Theory Study on the Mechanism of Iridium-Catalyzed Benzylamine C-H Alkenylation with Ethyl Acrylate. <i>ACS Omega</i> , 2020 , 5, 15446-15453	3.9	3
77	Theoretical elucidation of the multi-functional synthetic methodology for switchable Ni(0)-catalyzed C \equiv N allylations, alkenylations and dienylations with allenes. <i>Catalysis Science and Technology</i> , 2020 , 10, 4219-4228	5.5	6
76	Distinct Roles of Ag(I) and Cu(II) as Cocatalysts in Achieving Positional-Selective C-H Alkenylation of Isoxazoles: A Theoretical Investigation. <i>Journal of Organic Chemistry</i> , 2020 , 85, 8387-8396	4.2	5
75	Graphitic carbon nitride nanodots: electronic structure and its influence factors. <i>Journal of Materials Science</i> , 2020 , 55, 5488-5498	4.3	1
74	Substituent-controlled C-N coupling involved in Rh(III)-catalyzed oxidative [3+2] annulation of 2-acetyl-1-arylhidrazines with maleimides: A DFT study. <i>Journal of Organometallic Chemistry</i> , 2020 , 927, 121539	2.3	
73	Mechanism of Rh(III)-catalyzed alkylation of N-pyrimidylindoline with cyclopropanols: A DFT study. <i>Molecular Catalysis</i> , 2020 , 498, 111255	3.3	2
72	Theoretical Insights into Ester-Directed Reactions between Propiolates with 1,2-Benzisoxazoles by Au(I) Catalyst: [4 + 2]-Annulation versus Michael-Type Products. <i>Organometallics</i> , 2020 , 39, 4061-4068	3.8	2

71	Mechanism and Origin of Chemoselectivity of Ru-Catalyzed Cross-Coupling of Secondary Alcohols to β -Disubstituted Ketones. <i>Journal of Organic Chemistry</i> , 2020 , 85, 12444-12455	4.2	8
70	Mechanistic insights into the origin of substituent-directed product Z/E selectivity for gold-catalyzed [4+1]-annulations of 1,4-diyne-3-ols with isoxazoles: A DFT study. <i>Molecular Catalysis</i> , 2020 , 480, 110647	3.3	4
69	C-H Activation versus Ring Opening and Inner- versus Outer-Sphere Concerted Metalation-Deprotonation in Rh(III)-Catalyzed Oxidative Coupling of Oxime Ether and Cyclopropanol: A Density Functional Theory Study. <i>Journal of Organic Chemistry</i> , 2019 , 84, 11150-11160	4.2	10
68	A computational study on HS release and amide formation from thionoesters and cysteine. <i>Organic and Biomolecular Chemistry</i> , 2019 , 17, 5771-5778	3.9	2
67	Mechanistic Insights into the Ruthenium-Catalyzed [4 + 1] Annulation of Benzamides and Propargyl Alcohols by DFT Studies. <i>Organometallics</i> , 2019 , 38, 1877-1886	3.8	15
66	Mechanism and Origin of Stereoselectivity of Pd-Catalyzed Cascade Annulation of Aryl Halide, Alkene, and Carbon Monoxide via C-H Activation. <i>Journal of Organic Chemistry</i> , 2019 , 84, 4353-4362	4.2	7
65	C-H Acidity and Arene Nucleophilicity as Orthogonal Control of Chemoselectivity in Dual C-H Bond Activation. <i>Organic Letters</i> , 2019 , 21, 2360-2364	6.2	13
64	Mechanistic Investigation of Au(III)-Catalyzed Cycloisomerizations of N-Propargylcarboxamides. <i>European Journal of Organic Chemistry</i> , 2019 , 2019, 6822-6829	3.2	1
63	Mechanism and stereospecificity of Z-enamide synthesis from salicylaldehydes with isoxazoles using DFT calculations. <i>Journal of Organometallic Chemistry</i> , 2019 , 903, 120981	2.3	
62	The mechanism and structure-activity relationship of amide bond formation by silane derivatives: a computational study. <i>Organic and Biomolecular Chemistry</i> , 2019 , 17, 9232-9242	3.9	4
61	Mechanism of Cu-Catalyzed Aerobic C(CO) π H ₃ Bond Cleavage: A Combined Computational and Experimental Study. <i>ACS Catalysis</i> , 2019 , 9, 1066-1080	13.1	24
60	Mechanism and Rate-Determining Factors of Amide Bond Formation through Acyl Transfer of Mixed Carboxylic-Carbamic Anhydrides: A Computational Study. <i>Journal of Organic Chemistry</i> , 2018 , 83, 2676-2685	4.2	16
59	Mechanistic Unveiling of C=C Double-Bond Rotation and Origins of Regioselectivity and Product E/Z Selectivity of Pd-Catalyzed Olefinic C-H Functionalization of (E)-N-Methoxy Cinnamamide. <i>Journal of Organic Chemistry</i> , 2018 , 83, 2067-2076	4.2	12
58	Mechanism of N-to-S acyl transfer of N-(2-hydroxybenzyl) cysteine derivatives and origin of phenol acceleration effect. <i>Chinese Chemical Letters</i> , 2018 , 29, 1264-1268	8.1	10
57	A DFT mechanistic study on gold(I)-catalyzed cascade reaction of aminalkyne involving Petasis-Ferrier cyclization. <i>Journal of Organometallic Chemistry</i> , 2018 , 864, 136-142	2.3	2
56	Synthesis of indolines via a palladium/norbornene-catalyzed reaction of aziridines with aryl iodides. <i>Chemical Communications</i> , 2018 , 54, 3407-3410	5.8	48
55	Computational study of the mechanism of amide bond formation via CS-releasing 1,3-acyl transfer. <i>Organic and Biomolecular Chemistry</i> , 2018 , 16, 5808-5815	3.9	8
54	Mechanism of Palladium-Catalyzed Alkylation of Aryl Halides with Alkyl Halides through C β Activation: A Computational Study. <i>Organometallics</i> , 2018 , 37, 2222-2231	3.8	11

53	Mechanistic exploration of CpRe(CO) ₃ -catalyzed coupling of chloromethyloxirane with CO ₂ : Unexpected potentials of CO ligands. <i>Molecular Catalysis</i> , 2018 , 458, 25-32	3.3	1
52	Unveiling the mechanisms and secrets of chemoselectivities in Au(I)-catalyzed diazo-based couplings with aryl unsaturated aliphatic alcohols. <i>Catalysis Science and Technology</i> , 2018 , 8, 4450-4462	5.5	15
51	A Reaction Mechanism for Gold-Catalyzed Hydroamination/Cyclization of o-Phenyldiamine and Propargylic Alcohols. A DFT Study. <i>Organometallics</i> , 2018 , 37, 3035-3044	3.8	6
50	Boron Ester-Catalyzed Amidation of Carboxylic Acids with Amines: Mechanistic Rationale by Computational Study. <i>Chemistry - an Asian Journal</i> , 2018 , 13, 2685-2690	4.5	8
49	Mechanism and Origin of Et ₂ Al(OEt)-Induced Chemoselectivity of Nickel-Catalyzed Three-Component Coupling of One Diketene and Two Alkynes. <i>ACS Catalysis</i> , 2017 , 7, 1886-1896	13.1	33
48	Mechanism of trifluoroacetic-acid-promoted N-to-S acyl transfer of enamides. <i>Tetrahedron</i> , 2017 , 73, 4380-4386	2.4	7
47	A Ligand-Dissociation-Involved Mechanism in Amide Formation of Monofluoroacylboronates with Hydroxylamines. <i>Journal of Organic Chemistry</i> , 2017 , 82, 1064-1072	4.2	13
46	Theoretical Insight into C(sp ³)–B Bond Activations and Origins of Chemo- and Regioselectivities of Ir-Nickel-Mediated/-Catalyzed Couplings of 2-Trifluoromethyl-1-alkenes with Alkynes. <i>Organometallics</i> , 2017 , 36, 3739-3749	3.8	23
45	Mechanistic Study on Platinum-Catalyzed Domino Reaction of Benziodoxole and Pyrrole Homopropargylic Ethers for Indole Synthesis. <i>Organometallics</i> , 2017 , 36, 2843-2852	3.8	14
44	Mechanism of Amide Bond Formation from Carboxylic Acids and Amines Promoted by 9-Silafluorenyl Dichloride Derivatives. <i>Journal of Organic Chemistry</i> , 2017 , 82, 9087-9096	4.2	11
43	Theoretical study of the Cl-initiated atmospheric oxidation of methyl isopropenyl ketone. <i>RSC Advances</i> , 2017 , 7, 52801-52811	3.7	4
42	Mechanism of Pd-catalyzed acylation/alkenylation of aryl iodide: a DFT study. <i>Organic and Biomolecular Chemistry</i> , 2017 , 15, 6147-6156	3.9	20
41	Mechanistic investigation into Et ₃ N CH activation and chemoselectivity by Pd-Catalyzed intramolecular heck reaction of N-Vinylacetamides. <i>Journal of Organometallic Chemistry</i> , 2017 , 827, 56-66	2.3	14
40	Theoretical investigations on the interactions of glucokinase regulatory protein with fructose phosphates. <i>Computational Biology and Chemistry</i> , 2016 , 60, 21-31	3.6	1
39	Identification of the active site of human mitochondrial malonyl-coenzyme a decarboxylase: A combined computational study. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016 , 84, 792-802	4.2	1
38	Theoretical study on Pd-catalyzed reaction of aryl iodide with unsymmetrical alkyne. <i>Journal of Organometallic Chemistry</i> , 2016 , 803, 134-141	2.3	3
37	Mechanisms and origins of the switchable regioselectivity of FeBr ₃ -catalyzed [1,2]-aryl and [1,2]-alkyl shifts of α -aryl aldehydes. <i>Organic and Biomolecular Chemistry</i> , 2016 , 14, 2522-36	3.9	8
36	Theoretical study on Au(I)-catalyzed [2 + 2 + 2] cycloadditions of ynamides with two discrete nitriles. <i>Organic and Biomolecular Chemistry</i> , 2016 , 14, 2637-44	3.9	14

35	An efficient route to regioselective functionalization of benzo[b]thiophenes via palladium-catalyzed decarboxylative Heck coupling reactions: insights from experiment and computation. <i>Organic and Biomolecular Chemistry</i> , 2016 , 14, 895-904	3.9	10
34	Theoretical Study of Gold-Catalyzed Cyclization of 2-Alkynyl-N-propargylanilines and Rationalization of Kinetic Experimental Phenomena. <i>Journal of Organic Chemistry</i> , 2016 , 81, 9381-9388	4.2	27
33	Theoretical Insight into the Mechanisms and Regioselectivity of [4 + 3] and [4 + 1] Annulations of Enals with Azoalkenes Catalyzed by N-Heterocyclic Carbenes. <i>Journal of Organic Chemistry</i> , 2016 , 81, 9775-9784	4.2	30
32	Advances in theoretical study on transition-metal-catalyzed C≡C activation. <i>Science China Chemistry</i> , 2016 , 59, 1448-1466	7.9	42
31	Mechanistic insight into water-modulated cycloisomerization of enynyl esters using an Au(I) catalyst. <i>Dalton Transactions</i> , 2015 , 44, 5354-63	4.3	37
30	Mechanistic insight into conjugated N-N bond cleavage by Rh(III)-catalyzed redox-neutral C-H activation of pyrazolones. <i>Organic and Biomolecular Chemistry</i> , 2015 , 13, 8251-60	3.9	25
29	Strong chemisorption of CO on M@Bn _n (M = Co, Ir, Rh, Ru, Ta, Nb, n = 8-10) clusters: an implication for wheel boron clusters as CO gas detectors. <i>RSC Advances</i> , 2015 , 5, 82524-82530	3.7	8
28	Insight into Pd-catalyzed branching cyclizations of enediyne-imides towards furo[2,3-b]pyridines: a DFT study. <i>Organic and Biomolecular Chemistry</i> , 2015 , 13, 11539-49	3.9	8
27	Role of Acetate and Water in the Water-Assisted Pd(OAc) ₂ -Catalyzed Cross-Coupling of Alkenes with N-Tosyl Hydrazones: A DFT Study. <i>Organometallics</i> , 2014 , 33, 3453-3463	3.8	21
26	Theoretical Studies on a New Class of C-C Bond Formation: Palladium-Catalyzed Reactions of Diazocarbonyl Compounds with Allylic Esters. <i>Organometallics</i> , 2014 , 33, 1404-1415	3.8	20
25	Hydrothermal/thermal conversion synthesis of hierarchical porous MgO microrods as efficient adsorbents for lead(II) and chromium(VI) removal. <i>RSC Advances</i> , 2014 , 4, 30542-30550	3.7	23
24	Theoretical Investigation of the Controlled Metathesis Reactions of Methylruthenium(II) Complexes with Terminal Acetylenes. <i>European Journal of Inorganic Chemistry</i> , 2014 , 2014, 2502-2511	2.3	7
23	Molecular dynamics simulations of mutated Mycobacterium tuberculosis L-alanine dehydrogenase to illuminate the role of key residues. <i>Journal of Molecular Graphics and Modelling</i> , 2014 , 50, 61-70	2.8	5
22	Understanding the Reactions of Aryl Iodides with Alkynes to Give New C-C and C-I Bonds: A DFT Study. <i>Current Organic Chemistry</i> , 2014 , 18, 1661-1671	1.7	5
21	Theoretical studies on the interaction mechanisms between tetrachloro-p-benzoquinone and hydrogen peroxide. <i>Structural Chemistry</i> , 2013 , 24, 1253-1264	1.8	6
20	Theoretical investigation on Pt(II)- and Au(I)-mediated cycloisomerizations of propargylic 3-indoleacetate: [3 + 2]- versus [2 + 2]-cycloaddition products. <i>Organic and Biomolecular Chemistry</i> , 2013 , 11, 336-43	3.9	17
19	Theoretical Insight into PtCl ₂ -Catalyzed Isomerization of Cyclopropenes to Allenes. <i>Organometallics</i> , 2012 , 31, 4769-4778	3.8	13
18	A DFT STUDY OF CO MIGRATORY INSERTION REACTIONS WITH A NEW TYPE OF GROUP 10 METAL-ALKYL AND METAL-ALKOXIDE BONDS. <i>Journal of Theoretical and Computational Chemistry</i> , 2012 , 11, 1-17	1.8	7

17	Explorations of the nature of the coupling interactions between vitamin C and methylglyoxal: a DFT study. <i>Structural Chemistry</i> , 2011 , 22, 783-793	1.8	6
16	Preparation of Mesoporous ZnO Microspheres through a Membrane-Dispersion Microstructured Reactor and a Hydrothermal Treatment. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 13353-13361 ¹²	2.9	12
15	A DFT STUDY ON CO INSERTION AND C ₁ REDUCTIVE ELIMINATION INVOLVED IN THE CARBONYLATION OF METALLACYCLIC ZIRCONACENES. <i>Journal of Theoretical and Computational Chemistry</i> , 2011 , 10, 9-17	1.8	
14	Theoretical investigation on the isomerization reaction of 4-phenyl-hexa-1,5-enyne catalyzed by homogeneous Au catalysts. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 12893-9	2.8	32
13	Theoretical studies of the proton transfer behaviors in molecular complexes analogous to catalytic triad of serine protease: Toward understanding the existence and significance of the low-barrier hydrogen-bond in enzymatic catalysis. <i>Science in China Series B: Chemistry</i> , 2009 , 52, 131-136		2
12	Mechanisms of H ₂ , H ₂ C=CH ₂ , and O=CH ₂ Insertion into Cp ₂ Zr(η ⁵ -SiMe ₂ =NtBu)(PMe ₃). <i>European Journal of Inorganic Chemistry</i> , 2007 , 2007, 2046-2054	2.3	9
11	Theoretical study of magnetic coupling interaction in terephthalato-bridged Ni(II) binuclear systems. <i>International Journal of Quantum Chemistry</i> , 2004 , 97, 802-807	2.1	3
10	Structural modeling and magnetostructural correlations for heterobinuclear Cu(II)Ni(II) complex. <i>International Journal of Quantum Chemistry</i> , 2002 , 88, 347-354	2.1	3
9	Density Functional Studies of the Reactions of Lanthanide Monocations with Fluoromethane: C-F Bond Activation and Electron-Transfer Reactivity. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 4153-4157	2.8	26
8	Synthesis, Characterization and Antifungal Activity of Some Transition Metal Complexes of the Schiff Base Derived from 4-Acetylbi-Phenyl and S-Benzylidithiocarbazate. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , 1999 , 29, 1829-1841		4
7	Synthesis, Characterization of Cu(II) and Ni(II) Liquid Crystal Complexes of an Unsymmetrical β-Diketone Containing a Terminal Double Bond. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , 1999 , 29, 1283-1297		
6	Synthesis, Characterization of An Unsymmetrical Cu(II) Complex Liquid Crystal of a Schiff Base Containing a Terminal Double Bond. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , 1999 , 29, 1611-1624		
5	Synthesis and Characterization of a Pd-Coordinated Azo-Type Liquid Crystal. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , 1998 , 28, 1173-1185		1
4	Syntheses, Characterizations and Stabilities of some Transition Metal Complexes of 4-Acetylbi-phenyl Thiosemicarbazone. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , 1998 , 28, 1299-1312		3
3	Synthesis and Characterization of 2-Alkoxy-carbonylethyltin Trichlorides and their Complexes. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , 1997 , 27, 127-139		4
2	Transition Metal Complexes of the Benzoin Schiff Base of S-Benzylidithiocarbazate. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , 1997 , 27, 1115-1125		12
1	Synthesis and Characterization of Transition Metal Ternary Complexes of Glyoxylic Acid Thiosemicarbazone and 1,10-Phenanthroline. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , 1996 , 26, 1447-1454		7