

# Siwei Bi

## List of Publications by Year in descending order

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393982

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#	ARTICLE	IF	CITATIONS
1	Electronic Spin Moment As a Catalytic Descriptor for Fe Single-Atom Catalysts Supported on C <sub>2</sub> N. <i>Journal of the American Chemical Society</i> , 2021, 143, 4405-4413.	6.6	138
2	Synthesis of indolines <i>via</i> a palladium/norbornene-catalyzed reaction of aziridines with aryl iodides. <i>Chemical Communications</i> , 2018, 54, 3407-3410.	2.2	60
3	Advances in theoretical study on transition-metal-catalyzed C-H activation. <i>Science China Chemistry</i> , 2016, 59, 1448-1466.	4.2	47
4	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.	1.7	41
5	Mechanism and Origin of Et <sub>2</sub> Al(OEt)-Induced Chemoselectivity of Nickel-Catalyzed Three-Component Coupling of One Diketene and Two Alkynes. <i>ACS Catalysis</i> , 2017, 7, 1886-1896.	5.5	38
6	Mechanistic insight into water-modulated cycloisomerization of enynyl esters using an Au( <i>scpt</i> ) catalyst. <i>Dalton Transactions</i> , 2015, 44, 5354-5363.	1.6	37
7	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, 12893-12899.	1.1	33
8	Theoretical Study of Gold-Catalyzed Cyclization of 2-Alkynyl- <i>N</i> -propargylanilines and Rationalization of Kinetic Experimental Phenomena. <i>Journal of Organic Chemistry</i> , 2016, 81, 9381-9388.	1.7	30
9	Theoretical Insight into C(sp <sup>3</sup> )-F Bond Activations and Origins of Chemo- and Regioselectivities of Tunable Nickel-Mediated/Catalyzed Couplings of 2-Trifluoromethyl-1-alkenes with Alkynes. <i>Organometallics</i> , 2017, 36, 3739-3749.	1.1	30
10	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.	1.1	28
11	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.	1.7	28
12	Mechanistic insight into conjugated N-N bond cleavage by Rh( <i>scpt</i> )-catalyzed redox-neutral C-H activation of pyrazolones. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 8251-8260.	1.5	28
13	Mechanism of Cu-Catalyzed Aerobic C(CO)-CH <sub>3</sub> Bond Cleavage: A Combined Computational and Experimental Study. <i>ACS Catalysis</i> , 2019, 9, 1066-1080.	5.5	28
14	Mechanism of Pd-catalyzed acylation/alkenylation of aryl iodide: a DFT study. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 6147-6156.	1.5	27
15	Theoretical Studies on a New Class of C-C Bond Formation: Palladium-Catalyzed Reactions of $\pm$ -Diazocarbonyl Compounds with Allylic Esters. <i>Organometallics</i> , 2014, 33, 1404-1415.	1.1	25
16	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.	2.4	24
17	Mechanistic Insights into the Ruthenium-Catalyzed [4 + 1] Annulation of Benzamides and Propargyl Alcohols by DFT Studies. <i>Organometallics</i> , 2019, 38, 1877-1886.	1.1	23
18	Role of Acetate and Water in the Water-Assisted Pd(OAc) <sub>2</sub> -Catalyzed Cross-Coupling of Alkenes with <i>N</i> -Tosyl Hydrazones: A DFT Study. <i>Organometallics</i> , 2014, 33, 3453-3463.	1.1	22

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19	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.	1.7	20
20	Mechanism of Palladium-Catalyzed Alkylation of Aryl Halides with Alkyl Halides through C-H Activation: A Computational Study. <i>Organometallics</i> , 2018, 37, 2222-2231.	1.1	19
21	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.	1.7	18
22	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.	1.7	18
23	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, 336-343.	1.5	17
24	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.	1.5	17
25	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.	1.7	17
26	Mechanism and Origin of Chemoselectivity of Ru-Catalyzed Cross-Coupling of Secondary Alcohols to $\beta$ -Disubstituted Ketones. <i>Journal of Organic Chemistry</i> , 2020, 85, 12444-12455.	1.7	17
27	Theoretical study on Au(I)-catalyzed [2 + 2 + 2] cycloadditions of ynamides with two discrete nitriles. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 2637-2644.	1.5	16
28	Mechanistic Study on Platinum-Catalyzed Domino Reaction of Benziodoxole and Pyrrole Homopropargylic Ethers for Indole Synthesis. <i>Organometallics</i> , 2017, 36, 2843-2852.	1.1	15
29	Mechanistic investigation into Et <sub>3</sub> N C-H activation and chemoselectivity by Pd-Catalyzed intramolecular Heck reaction of N-vinylacetamides. <i>Journal of Organometallic Chemistry</i> , 2017, 827, 56-66.	0.8	15
30	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.	2.1	15
31	Transition Metal Complexes of the Benzoin Schiff Base of S-Benzylidithiocarbamate. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , 1997, 27, 1115-1125.	1.8	13
32	Theoretical Insight into PtCl <sub>2</sub> -Catalyzed Isomerization of Cyclopropenes to Allenes. <i>Organometallics</i> , 2012, 31, 4769-4778.	1.1	13
33	A Ligand-Dissociation-Involved Mechanism in Amide Formation of Monofluoroacylboronates with Hydroxylamines. <i>Journal of Organic Chemistry</i> , 2017, 82, 1064-1072.	1.7	13
34	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.	1.7	13
35	Preparation of Mesoporous ZnO Microspheres through a Membrane-Dispersion Microstructured Reactor and a Hydrothermal Treatment. <i>Industrial &amp; Engineering Chemistry Research</i> , 2011, 50, 13355-13361.	1.8	12
36	Mechanisms and origins of the switchable regioselectivity of FeBr <sub>3</sub> -catalyzed [1,2]-aryl and [1,2]-alkyl shifts of $\alpha$ -aryl aldehydes. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 2522-2536.	1.5	10

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37	Mechanism of N-to-S acyl transfer of N-(2-hydroxybenzyl) cysteine derivatives and origin of phenol acceleration effect. Chinese Chemical Letters, 2018, 29, 1264-1268.	4.8	10
38	Boron Esterâ€Catalyzed Amidation of Carboxylic Acids with Amines: Mechanistic Rationale by Computational Study. Chemistry - an Asian Journal, 2018, 13, 2685-2690.	1.7	10
39	Computational study of the mechanism of amide bond formation <i>via</i> CS <sub>2</sub> -releasing 1,3-acyl transfer. Organic and Biomolecular Chemistry, 2018, 16, 5808-5815.	1.5	10
40	The mechanism and structureâ€“activity relationship of amide bond formation by silane derivatives: a computational study. Organic and Biomolecular Chemistry, 2019, 17, 9232-9242.	1.5	10
41	Mechanisms of H <sub>2</sub> , H <sub>2</sub> C=CH <sub>2</sub> , and O=CH <sub>2</sub> Insertion into Cp <sub>2</sub> Zr( $\eta$ -2-SiMe <sub>2</sub> =NtBu)(PMe <sub>3</sub> ). European Journal of Inorganic Chemistry, 2007, 2007, 2046-2054.	1.0	9
42	Strong chemisorption of CO on M@B <sub>n</sub> (M = Co, Ir, Rh, Ru, Ta, Nb, $n=1-10$ ). Tj ETQq0 0 0 rgBT /Overlock 10 82524-82530.	1.7	9
43	Insight into Pd-catalyzed branching cyclizations of enediyne-imides towards furo[2,3-b]pyridines: a DFT study. Organic and Biomolecular Chemistry, 2015, 13, 11539-11549.	1.5	9
44	Distinct Roles of Ag(I) and Cu(II) as Cocatalysts in Achieving Positional-Selective Câ€“H Alkenylation of Isoxazoles: A Theoretical Investigation. Journal of Organic Chemistry, 2020, 85, 8387-8396.	1.7	9
45	A DFT STUDY OF CO MIGRATORY INSERTION REACTIONS WITH A NEW TYPE OF GROUP 10 METAL-ALKYL AND METAL-ALKOXIDE BONDS. Journal of Theoretical and Computational Chemistry, 2012, 11, 1-17.	1.8	8
46	Molecular dynamics simulations of mutated Mycobacterium tuberculosis l-alanine dehydrogenase to illuminate the role of key residues. Journal of Molecular Graphics and Modelling, 2014, 50, 61-70.	1.3	8
47	A Reaction Mechanism for Gold-Catalyzed Hydroamination/Cyclization of <i>o</i> -Phenylendiamine and Propargylic Alcohols. A DFT Study. Organometallics, 2018, 37, 3035-3044.	1.1	8
48	Mechanism and Origin of Stereoselectivity of Pd-Catalyzed Cascade Annulation of Aryl Halide, Alkene, and Carbon Monoxide via Câ€“H Activation. Journal of Organic Chemistry, 2019, 84, 4353-4362.	1.7	8
49	Theoretical elucidation of the multi-functional synthetic methodology for switchable Ni(0)-catalyzed Câ€“H allylations, alkenylations and dienylations with allenes. Catalysis Science and Technology, 2020, 10, 4219-4228.	2.1	8
50	Synthesis and Characterization of Transition Metal Ternary Complexes of Glyoxylic Acid Thiosemicarbazone and 1,10-Phenanthroline. Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry, 1996, 26, 1447-1454.	1.8	7
51	Explorations of the nature of the coupling interactions between vitamin C and methylglyoxal: a DFT study. Structural Chemistry, 2011, 22, 783-793.	1.0	7
52	Theoretical Investigation of the Controlled Metathesis Reactions of Methylruthenium(II) Complexes with Terminal Acetylenes. European Journal of Inorganic Chemistry, 2014, 2014, 2502-2511.	1.0	7
53	Mechanism of trifluoroacetic-acid-promoted N-to-S acyl transfer of enamides. Tetrahedron, 2017, 73, 4380-4386.	1.0	7
54	Synthesis and Characterization of 2-Alkoxy-carbonyl-ethyltin Trichlorides and their Complexes. Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry, 1997, 27, 127-139.	1.8	6

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55	Theoretical studies on the interaction mechanisms between tetrachloro-p-benzoquinone and hydrogen peroxide. <i>Structural Chemistry</i> , 2013, 24, 1253-1264.	1.0	6
56	Theoretical study of the Cl-initiated atmospheric oxidation of methyl isopropenyl ketone. <i>RSC Advances</i> , 2017, 7, 52801-52811.	1.7	6
57	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.	1.0	5
58	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.	2.2	5
59	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.	1.3	5
60	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.	1.3	5
61	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.	1.1	5
62	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.	0.9	5
63	Synthesis, Characterization and Antifungal Activity of Some Transition Metal Complexes of the Schiff Base Derived from 4-Acetylbi-Phenyl and S-Benzylthiocarbamate. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , 1999, 29, 1829-1841.	1.8	4
64	Theoretical study on Pd-catalyzed reaction of aryl iodide with unsymmetrical alkyne. <i>Journal of Organometallic Chemistry</i> , 2016, 803, 134-141.	0.8	4
65	Mechanism of Rh(III)-catalyzed alkylation of N-pyrimidylindoline with cyclopropanols: A DFT study. <i>Molecular Catalysis</i> , 2020, 498, 111255.	1.0	4
66	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.	1.1	4
67	Density Functional Theory Study on the Mechanism of Iridium-Catalyzed Benzylamine <i>ortho</i> C-H Alkenylation with Ethyl Acrylate. <i>ACS Omega</i> , 2020, 5, 15446-15453.	1.6	4
68	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.	1.7	4
69	Noncovalent Interaction- and Steric Effect-Controlled Regiodivergent Selectivity in Dimeric Manganese-Catalyzed Hydroarylation of Internal Alkynes: A Computational Study. <i>Journal of Organic Chemistry</i> , 2022, 87, 4215-4225.	1.7	4
70	Syntheses, Characterizations and Stabilities of some Transition Metal Complexes of 4-Acetylbiphenyl Thiosemicarbazone. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , 1998, 28, 1299-1312.	1.8	3
71	Structural modeling and magnetostructural correlations for heterobinuclear Cu(II)-Ni(II) complex. <i>International Journal of Quantum Chemistry</i> , 2002, 88, 347-354.	1.0	3
72	Theoretical study of magnetic coupling interaction in terephthalato-bridged Ni(II) binuclear systems. <i>International Journal of Quantum Chemistry</i> , 2004, 97, 802-807.	1.0	3

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73	Mechanistic Investigation of Au(III)-Catalyzed Cycloisomerizations of <i>N</i> -Propargylcarboxamides. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 6822-6829.	1.2	3
74	A computational study on H <sub>2</sub> S release and amide formation from thionoesters and cysteine. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 5771-5778.	1.5	3
75	Graphitic carbon nitride nanodots: electronic structure and its influence factors. <i>Journal of Materials Science</i> , 2020, 55, 5488-5498.	1.7	3
76	Decarbonylative Issues Involved in Ru(II)-Catalyzed [6+2] Annulation Reaction of Hydroxychromone with Alkyne: A DFT Study. <i>European Journal of Organic Chemistry</i> , 2021, 2021, 266-273.	1.2	3
77	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.	0.8	2
78	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.	1.5	2
79	A DFT mechanistic study on gold(I)-catalyzed cascade reaction of aminaloalkyne involving Petasis-Ferrier cyclization. <i>Journal of Organometallic Chemistry</i> , 2018, 864, 136-142.	0.8	2
80	Mechanistic exploration of CpRe(CO) <sub>3</sub> -catalyzed coupling of chloromethyloxirane with CO <sub>2</sub> : Unexpected potentials of CO ligands. <i>Molecular Catalysis</i> , 2018, 458, 25-32.	1.0	2
81	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.	1.8	1
82	Synthesis, Characterization of Cu(II) and Ni(II) Liquid Crystal Complexes of an Unsymmetrical $\beta$ -Diketone Containing a Terminal Double Bond. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , 1999, 29, 1283-1297.	1.8	1
83	Theoretical investigations on the interactions of glucokinase regulatory protein with fructose phosphates. <i>Computational Biology and Chemistry</i> , 2016, 60, 21-31.	1.1	1
84	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.	1.6	1
85	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.	1.0	1
86	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.	1.8	0
87	A DFT STUDY ON CO INSERTION AND $\alpha$ -REDUCTIVE ELIMINATION INVOLVED IN THE CARBONYLATION OF METALLACYCLIC ZIRCONACENES. <i>Journal of Theoretical and Computational Chemistry</i> , 2011, 10, 9-17.	1.8	0
88	Mechanism and stereospecificity of Z-enamide synthesis from salicylaldehydes with isoxazoles using DFT calculations. <i>Journal of Organometallic Chemistry</i> , 2019, 903, 120981.	0.8	0
89	Substituent-controlled C-N coupling involved in Rh(III)-catalyzed oxidative [3+2] annulation of 2-acetyl-1-arylhydrazines with maleimides: A DFT study. <i>Journal of Organometallic Chemistry</i> , 2020, 927, 121539.	0.8	0