Zhi-Xiang Wang

List of Publications by Year
in descending order

106 papers	3,973 citations	109321 35 h-index	138484 58 g-index
108 all docs	108 docs citations	108 times ranked	3105 citing authors

#	Article	IF	Citations
1	The Catalytic Role of N-Heterocyclic Carbene in a Metal-Free Conversion of Carbon Dioxide into Methanol: A Computational Mechanism Study. Journal of the American Chemical Society, 2010, 132, 12388-12396.	13.7	235
2	Four Decades of the Chemistry of Planar Hypercoordinate Compounds. Angewandte Chemie - International Edition, 2015, 54, 9468-9501.	13.8	217
3	Catalytic Mechanisms of Direct Pyrrole Synthesis via Dehydrogenative Coupling Mediated by PNP-Ir or PNN-Ru Pincer Complexes: Crucial Role of Proton-Transfer Shuttles in the PNP-Ir System. Journal of the American Chemical Society, 2014, 136, 4974-4991.	13.7	171
4	How Does the Nickel Pincer Complex Catalyze the Conversion of CO₂ to a Methanol Derivative? A Computational Mechanistic Study. Inorganic Chemistry, 2011, 50, 3816-3825.	4.0	159
5	Computational Study on the Catalytic Role of Pincer Ruthenium(II)-PNN Complex in Directly Synthesizing Amide from Alcohol and Amine: The Origin of Selectivity of Amide over Ester and Imine. Organometallics, 2011, 30, 5233-5247.	2.3	149
6	A Computational Mechanistic Study of an Unprecedented Heck-Type Relay Reaction: Insight into the Origins of Regio- and Enantioselectivities. Journal of the American Chemical Society, 2014, 136, 986-998.	13.7	118
7	CAl4Be and CAl3Be2â^': global minima with a planar pentacoordinate carbon atom. Chemical Communications, 2010, 46, 8776.	4.1	104
8	Palladium-Catalyzed Câ€“H Functionalization of Acyldiazomethane and Tandem Cross-Coupling Reactions. Journal of the American Chemical Society, 2015, 137, 4435-4444.	13.7	94
9	Gold catalyzed hydrogenations of small imines and nitriles: enhanced reactivity of Au surface toward H₂via collaboration with a Lewis base. Chemical Science, 2014, 5, 1082-1090.	7.4	91
10	Computational Mechanistic Study of Fe-Catalyzed Hydrogenation of Esters to Alcohols: Improving Catalysis by Accelerating Precatalyst Activation with a Lewis Base. ACS Catalysis, 2014, 4, 4377-4388.	11.2	91
11	Computational Insight into the Mechanism of Selective Imine Formation from Alcohol and Amine Catalyzed by the Ruthenium(II)â€PNP Pincer Complex. European Journal of Inorganic Chemistry, 2012, 2012, 5011-5020.	2.0	79
12	Computational Mechanistic Study of the Hydrogenation of Carbonate to Methanol Catalyzed by the Ru^{II}PNN Complex. Inorganic Chemistry, 2012, 51, 5716-5727.	4.0	77
13	The orthoâ€Difluoroalkylation of Aryliodanes with Enol Silyl Ethers: Rearrangement Enabled by a Fluorine Effect. Angewandte Chemie - International Edition, 2019, 58, 5956-5961.	13.8	75
14	Hydrogenation of Esters Catalyzed by Ruthenium PN³-Pincer Complexes Containing an Aminophosphine Arm. Organometallics, 2014, 33, 4152-4155.	2.3	74
15	Mechanism of the Methyltrioxorheniumâ€Catalyzed Deoxydehydration of Polyols: A New Pathway Revealed. Chemistry - A European Journal, 2013, 19, 3827-3832.	3.3	71
16	Visibleâ€Lightâ€Induced Selective Photolysis of Phosphonium Iodide Salts for Monofluoromethylations. Angewandte Chemie - International Edition, 2021, 60, 25477-25484.	13.8	69
17	Mechanistic Insight into Ketone Î±-Alkylation with Unactivated Olefins via Câ€“H Activation Promoted by Metalâ€“Organic Cooperative Catalysis (MOCC): Enriching the MOCC Chemistry. Journal of the American Chemical Society, 2015, 137, 6279-6291.	13.7	66
18	Density Functional Theory Mechanistic Study of the Reduction of CO₂ to CH₄ Catalyzed by an Ammonium Hydridoborate Ion Pair: CO₂ Activation via Formation of a Formic Acid Entity. Inorganic Chemistry, 2013, 52, 12098-12107.	4.0	65

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19	Unveiling Secrets of Overcoming the â€œHeteroatom Problemâ€•in Palladium-Catalyzed Aerobic Câ€“H Functionalization of Heterocycles: A DFT Mechanistic Study. Journal of the American Chemical Society, 2016, 138, 2712-2723.	13.7	65
20	Computationally Designed Metal-Free Hydrogen Activation Site: Reaching the Reactivity of Metalâˆ’Ligand Bifunctional Hydrogenation Catalysts. Inorganic Chemistry, 2010, 49, 295-301.	4.0	61
21	D3h CN3Be3+ and CO3Li3+: viable planar hexacoordinate carbon prototypes. Physical Chemistry Chemical Physics, 2012, 14, 14760.	2.8	59
22	A Thorough DFT Study of the Mechanism of Homodimerization of Terminal Olefins through Metathesis with a Chelated Ruthenium Catalyst: From Initiation to Z Selectivity to Regeneration. Organometallics, 2012, 31, 7222-7234.	2.3	58
23	Diverse catalytic reactivity of a dearomatized PN³P*â€“nickel hydride pincer complex towards CO₂ reduction. Chemical Communications, 2018, 54, 11395-11398.	4.1	56
24	Does the Ruthenium Nitrato Catalyst Work Differently in Z-Selective Olefin Metathesis? A DFT Study. Organometallics, 2012, 31, 8654-8657.	2.3	52
25	Gold-Catalyzed Atom-Economic Synthesis of Sulfone-Containing Pyrrolo[2,1-a]isoquinolines from Diynamides: Evidence for Consecutive Sulfonyl Migration. ACS Catalysis, 2019, 9, 2610-2617.	11.2	49
26	Selective ortho Câˆ’H Cyanoalkylation of (Diacetoxyiodo)arenes through [3,3]â€Sigmatropic Rearrangement. Angewandte Chemie - International Edition, 2018, 57, 9078-9082.	13.8	47
27	Selective [5,5]â€Sigmatropic Rearrangement by Assembly of Aryl Sulfoxides with Allyl Nitriles. Angewandte Chemie - International Edition, 2019, 58, 5316-5320.	13.8	47
28	Depolymerization of Oxidized Lignin Catalyzed by Formic Acid Exploits an Unconventional Elimination Mechanism Involving 3câ€“4e Bonding: A DFT Mechanistic Study. ACS Catalysis, 2015, 5, 6386-6396.	11.2	46
29	Computational design of metal-free catalysts for catalytic hydrogenation of imines. Dalton Transactions, 2010, 39, 4038.	3.3	45
30	Reaction Mechanism of Phosphaneâ€Catalyzed [4+2] Annulations between Î±â€Alkylallenoates and Activated Alkenes: A Computational Study. European Journal of Organic Chemistry, 2012, 2012, 3587-3597.	2.4	45
31	Insight into the relative reactivity of â€œFrustrated Lewis pairsâ€•and stable carbenes in activating H2 and CH4: A comparative computational study. Physical Chemistry Chemical Physics, 2010, 12, 5268.	2.8	44
32	Planar Tetracoordinate Carbon Species Involving Beryllium Substituents. Inorganic Chemistry, 2008, 47, 1332-1336.	4.0	42
33	Encumbering the intramolecular Ï€ donation by using a bridge: A strategy for designing metal-free compounds to hydrogen activation. Science Bulletin, 2010, 55, 239-245.	1.7	38
34	Computationally Designed Families of Flat, Tubular, and Cage Molecules Assembled with â€œStarbeneneâ€• Building Blocks through Hydrogenâ€Bridge Bonds. Chemistry - A European Journal, 2010, 16, 1271-1280.	3.3	38
35	Catalytic metal-free ketone hydrogenation: a computational experiment. Dalton Transactions, 2010, 39, 5519.	3.3	38
36	Alkynyl Sulfonium Salts Can Be Employed as Chalcogenâ€Bonding Catalysts and Generate Alkynyl Radicals under Blueâ€Light Irradiation. Angewandte Chemie - International Edition, 2022, 61, .	13.8	36

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37	Reversible Heterolytic Methane Activation of Metalâ€Free Closedâ€Shell Molecules: A Computational Proofâ€ofâ€Principle Study. European Journal of Inorganic Chemistry, 2010, 2010, 2254-2260.	2.0	35
38	Designing Metalâ€Free Catalysts by Mimicking Transitionâ€Metal Pincer Templates. Chemistry - A European Journal, 2011, 17, 2038-2043.	3.3	34
39	Asymmetric Iodonio-[3,3]-Sigmatropic Rearrangement to Access Chiral Î±-Aryl Carbonyl Compounds. Journal of the American Chemical Society, 2020, 142, 6884-6890.	13.7	32
40	Photochemical Decarboxylative C(sp³)â€“X Coupling Facilitated by Weak Interaction of N-Heterocyclic Carbene. Organic Letters, 2020, 22, 8059-8064.	4.6	30
41	Formylation or methylation: what determines the chemoselectivity of the reaction of amine, CO₂, and hydrosilane catalyzed by 1,3,2-diazaphospholene?. Chemical Science, 2017, 8, 7637-7650.	7.4	28
42	Differences between the elimination of early and late transition metals: DFT mechanistic insights into the titanium-catalyzed synthesis of pyrroles from alkynes and diazenes. Chemical Science, 2017, 8, 2413-2425.	7.4	27
43	Mechanism and Origins of Z Selectivity of the Catalytic Hydroalkoxylation of Alkynes via Rhodium Vinylidene Complexes To Produce Enol Ethers. Organometallics, 2013, 32, 2804-2813.	2.3	26
44	Visible-Light-Triggered Iodinations Facilitated by Weak Electrostatic Interaction of N-Heterocyclic Carbenes. Organic Letters, 2020, 22, 7187-7192.	4.6	26
45	Metal-free catalysts for hydrogenation of both small and large imines: a computational experiment. Dalton Transactions, 2011, 40, 1929.	3.3	25
46	Reductive ortho Câ€“H cyanoalkylation of aryl(heteroaryl) sulfoxides: a general approach to Î±-aryl(heteroaryl) nitriles. Organic Chemistry Frontiers, 2018, 5, 1756-1762.	4.5	25
47	A comparative DFT study of TBD-catalyzed reactions of amines with CO₂ and hydrosilane: the effect of solvent polarity on the mechanistic preference and the origins of chemoselectivities. Chemical Communications, 2018, 54, 10870-10873.	4.1	25
48	DFT Mechanistic Account for the Site Selectivity of Electron-Rich C(sp³)â€“H Bond in the Manganese-Catalyzed Aminations. Organic Letters, 2020, 22, 453-457.	4.6	25
49	Palladium-Catalyzed Three-Component Coupling Reaction of o-Bromobenzaldehyde, N-Tosylhydrazone, and Methanol. Organic Letters, 2020, 22, 2087-2092.	4.6	25
50	Palladium-Catalyzed Reductive Cross-Coupling Reaction of Aryl Chromium(0) Fischer Carbene Complexes with Aryl Iodides. Organometallics, 2018, 37, 1-10.	2.3	24
51	Density Functional Theory Mechanistic Insight into the Base-Free Nickel-Catalyzed Suzukiâ€“Miyaura Cross-Coupling of Acid Fluoride: Concerted versus Stepwise Transmetalation. Journal of Organic Chemistry, 2019, 84, 13983-13991.	3.2	24
52	Catalytic metal-free intramolecular hydroaminations of non-activated aminoalkenes: A computational exploration. Dalton Transactions, 2012, 41, 9091.	3.3	23
53	Semi-interpenetrating-network all-solid-state polymer electrolyte with liquid crystal constructing efficient ion transport channels for flexible solid lithium-metal batteries. Journal of Energy Chemistry, 2022, 67, 157-167.	12.9	23
54	Computational mechanistic studies of acceptorless dehydrogenation reactions catalyzed by transition metal complexes. Science China Chemistry, 2012, 55, 1991-2008.	8.2	22

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55	Selective ortho Câ^'H Cyanoalkylation of (Diacetoxyiodo)arenes through [3,3]â€Sigmatropic Rearrangement. Angewandte Chemie, 2018, 130, 9216-9220.	2.0	22
56	Photoinduced Î±-Alkenylation of Katritzky Salts: Synthesis of Î²,Î³-Unsaturated Esters. Organic Letters, 2021, 23, 1577-1581.	4.6	22
57	A donorâ€“acceptor complex enables the synthesis of E-olefins from alcohols, amines and carboxylic acids. Chemical Science, 2021, 12, 6684-6690.	7.4	22
58	Assessing the performance of commonly used DFT functionals in studying the chemistry of frustrated Lewis pairs. Journal of Theoretical and Computational Chemistry, 2014, 13, 1350074.	1.8	21
59	Viable aromatic Be_nH_n stars enclosing a planar hypercoordinate boron or late transition metal. Physical Chemistry Chemical Physics, 2018, 20, 7217-7222.	2.8	21
60	A Pseudodearomatized PN³P*Niâ€“H Complex as a Ligand and Ïƒ-Nucleophilic Catalyst. Journal of Organic Chemistry, 2018, 83, 14969-14977.	3.2	21
61	Zâ€Selective Î±â€Arylation of Î±,Î²â€Unsaturated Nitriles via [3,3]â€Sigmatropic Rearrangement. Angewandte Chemie - International Edition, 2021, 60, 2339-2345.	13.8	21
62	Additive-Free, Visible-Light-Enabled Decarboxylative Alkylation of Enamides. Organic Letters, 2021, 23, 8262-8266.	4.6	21
63	Mechanism of Z-Selective Olefin Metathesis Catalyzed by a Ruthenium Monothiolate Carbene Complex: A DFT Study. Organometallics, 2014, 33, 4290-4294.	2.3	20
64	A DFT study unveils the secret of how H₂ is activated in the N-formylation of amines with CO₂ and H₂ catalyzed by Ru(<scp>ii</scp>) pincer complexes in the absence of exogenous additives. Chemical Communications, 2017, 53, 12148-12151.	4.1	18
65	Red-emissive poly(phenylene vinylene)-derivated semiconductors with well-balanced ambipolar electrical transporting properties. Journal of Materials Chemistry C, 2020, 8, 10868-10879.	5.5	18
66	Density Functional Theory Mechanistic Study of Ni-Catalyzed Reductive Alkyneâ€“Alkyne Cyclodimerization: Oxidative Cyclization versus Outer-Sphere Proton Transfer. Organic Letters, 2020, 22, 2454-2459.	4.6	18
67	How Does an Earth-Abundant Copper-Based Catalyst Achieve Anti-Markovnikov Hydrobromination of Alkynes? A DFT Mechanistic Study. Organometallics, 2016, 35, 1923-1930.	2.3	16
68	N-Heterocyclic Nitreniums Can Be Employed as Photoredox Catalysts for the Single-Electron Reduction of Aryl Halides. Organic Letters, 2022, 24, 4598-4602.	4.6	16
69	The orthoâ€Difluoroalkylation of Aryliodanes with Enol Silyl Ethers: Rearrangement Enabled by a Fluorine Effect. Angewandte Chemie, 2019, 131, 6017-6022.	2.0	15
70	Understanding the Chemoselectivity in Palladium-Catalyzed Three-Component Reaction of o-Bromobenzaldehyde, N-Tosylhydrazone, and Methanol. Organic Letters, 2020, 22, 3251-3257.	4.6	15
71	System: A DFT Mechanistic Study. Organic Letters, 2021, 23, 1535-1540.	4.6	15
72	Donorâ€“Acceptor Complex Enables Cascade Radical Cyclization of N-Arylacrylamides with Katritzky Salts. Organic Letters, 2021, 23, 5425-5429.	4.6	15

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73	How accurate are the popular PCM/GB continuum solvation models for calculating the solvation energies of amino acid side-chain analogs?. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	14
74	Linear, planar, and tubular molecular structures constructed by double planar tetracoordinate carbon D₂_h C₂(BeH)₄ species via hydrogenâ€bridged ï£¿BeH₂Beï£¿ bonds. Journal of Computational Chemistry, 2016, 37, 261-269.	3.3	14
75	Selective [5,5]â€Sigmatropic Rearrangement by Assembly of Aryl Sulfoxides with Allyl Nitriles. Angewandte Chemie, 2019, 131, 5370-5374.	2.0	14
76	A Unified Mechanism to Account for Manganeseâ€or Rutheniumâ€Catalyzed Nitrile Î±â€Olefinations by Primary or Secondary Alcohols: A DFT Mechanistic Study. Chemistry - A European Journal, 2019, 25, 3939-3949.	3.3	14
77	Site-Selective Pyridyl Alkyl Ketone Synthesis from N-Alkenoxypyridiniums through Boekelheide-Type Rearrangements. Organic Letters, 2020, 22, 5617-5621.	4.6	13
78	Visible-light-induced N-heterocyclic carbene mediated cascade transformation of N-alkenoxypyridinium salts. Chinese Chemical Letters, 2022, 33, 4298-4302.	9.0	13
79	Strong Preference of the Redoxâ€Neutral Mechanism over the Redox Mechanism for the Ti^{IV} Catalysis Involved in the Carboamination of Alkyne with Alkene and Diazene. Chemistry - A European Journal, 2018, 24, 7010-7025.	3.3	12
80	Manipulation of the Reducibility of Ceriaâ€Supported Au Catalysts by Interface Engineering. ChemCatChem, 2013, 5, 1308-1312.	3.7	11
81	DFT mechanistic study of the H₂-assisted chain transfer copolymerization of propylene andp-methylstyrene catalyzed by zirconocene complex. Journal of Polymer Science Part A, 2015, 53, 576-585.	2.3	10
82	Zigzag double-chain Câ€“Be nanoribbon featuring planar pentacoordinate carbons and ribbon aromaticity. Journal of Materials Chemistry C, 2017, 5, 408-414.	5.5	10
83	Moritaâ€“Baylisâ€“Hillmanâ€Type [3,3]â€Rearrangement: Switching fromZâ€toEâ€Selective Î±â€Arylation by New Rearrangement Partners. Angewandte Chemie - International Edition, 2021, 60, 11414-11422.	13.8	10
84	DFT insight into asymmetric alkylâ€“alkyl bond formation via nickel-catalysed enantioconvergent reductive coupling of racemic electrophiles with olefins. Chemical Science, 2022, 13, 3728-3739.	7.4	9
85	Divergent isoindolinone synthesis through palladium-catalyzed isocyanide bridging Câ€“H activation. Cell Reports Physical Science, 2022, 3, 100776.	5.6	9
86	Computational Design of Metal-Free Molecules for Activation of Small Molecules, Hydrogenation, and Hydroamination. Topics in Current Chemistry, 2012, 332, 231-266.	4.0	8
87	Highly enantioselective 1,6-addition of dienolates to coumarins and chromones through N-heterocyclic carbene catalysis. Organic Chemistry Frontiers, 2020, 7, 3692-3697.	4.5	8
88	How does the nickel catalyst control the doubly enantioconvergent coupling of racemic alkyl nucleophiles and electrophiles? The rebound mechanism. Organic Chemistry Frontiers, 2020, 7, 3411-3419.	4.5	8
89	DFT Mechanistic Insight into the Dioxygenase-like Reactivity of a Co^{III}-peroxo Complex: Oâ€“O Bond Cleavage via a [1,3]-Sigmatropic Rearrangement-like Mechanism. Inorganic Chemistry, 2020, 59, 2051-2061.	4.0	8
90	Visibleâ€Lightâ€Induced Selective Photolysis of Phosphonium Iodide Salts for Monofluoromethylations. Angewandte Chemie, 2021, 133, 25681-25688.	2.0	8

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91	Alkynyl Sulfonium Salts Can Be Employed as Chalcogenâ€Bonding Catalysts and Generate Alkynyl Radicals under Blueâ€Light Irradiation. Angewandte Chemie, 2022, 134, .	2.0	8
92	The Origins of the Differences between Alkyne Hydroalkoxylations Catalyzed by 8â€Quinolinolatoâ€•and Dipyrrinatoâ€Ligated Rh^I Complexes: A DFT Mechanistic Study. European Journal of Inorganic Chemistry, 2017, 2017, 2713-2722.	2.0	7
93	Pyrylium salts acting as both energy transfer and electron transfer photocatalysts for E â†' Z isomerization of activated alkenes and cyclization of cinnamic or biaryl carboxylic acids. Organic Chemistry Frontiers, 2022, 9, 973-978.	4.5	7
94	Metal-free homolytic hydrogen activation: a quest through density functional theory computations. New Journal of Chemistry, 2016, 40, 8141-8148.	2.8	6
95	Noncovalent Molecular Heterojunction: Structure Determination and Property Characterization using Scanning Tunneling Microscopy/Spectroscopy and Theoretical Calculations. Journal of Physical Chemistry C, 2017, 121, 13701-13706.	3.1	6
96	Computational mechanistic study of Ru-catalyzed CO₂ reduction by pinacolborane revealing the Ïƒâ€“Ï€ coupling mechanism for CO₂ decarbonylation. Dalton Transactions, 2018, 47, 4804-4819.	3.3	6
97	DFT Study of PNP-Mn-Catalyzed Acceptorless Dehydrogenative Coupling of Primary Alcohols with Hydrazine to Give Alkene or Azine. Organometallics, 2019, 38, 3590-3601.	2.3	6
98	Water facilitated photolysis of perfluoroalkyl iodides via halogen bonding. Organic Chemistry Frontiers, 0, , .	4.5	6
99	DFT Mechanistic Insights into Aldehyde Deformylations with Biomimetic Metalâ€“Dioxygen Complexes: Distinct Mechanisms and Reaction Rules. Jacs Au, 2022, 2, 745-761.	7.9	6
100	D3h [A-CE3-A]â^' (E = Al and Ga, A = Si, Ge, Sn, and Pb): A new class of hexatomic mono-anionic species with trigonal bipyramidal carbon. Journal of Chemical Physics, 2014, 140, 104302.	3.0	5
101	Î±-Câ€“H difluoroalkylation of alkyl sulfoxides via intermolecular Pummerer reaction. Organic Chemistry Frontiers, 2021, 8, 1280-1287.	4.5	5
102	Differences between insertions of ethylene into metallocene and nonâ€•metallocene ethylene polymerization catalysts. Journal of Physical Organic Chemistry, 2013, 26, 70-76.	1.9	4
103	A strategy for developing metal-free hydrogenation catalysts: a DFT proof-of-principle study. Dalton Transactions, 2018, 47, 7709-7714.	3.3	4
104	Z â€Selective Î±â€•Arylation of Î±,Î²â€Unsaturated Nitriles via [3,3]â€Sigmatropic Rearrangement. Angewandte Chemie, 2021, 133, 2369-2375.	2.0	4
105	Moritaâ€“Baylisâ€“Hillmanâ€•Type [3,3]â€Rearrangement: Switching from Z â€•to E â€Selective Î±â€•Arylation by New Rearrangement Partners. Angewandte Chemie, 2021, 133, 11515-11523.	2.0	2
106	Innentitelbild: Alkynyl Sulfonium Salts Can Be Employed as Chalcogenâ€Bonding Catalysts and Generate Alkynyl Radicals under Blueâ€Light Irradiation (Angew. Chem. 16/2022). Angewandte Chemie, 2022, 134, .	2.0	0