

Yun-Fang Yang

List of Publications by Year in descending order

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66
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4,110
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168829

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#	ARTICLE	IF	CITATIONS
1	Computational insights into different regioselectivities in the Ir-porphyrin-catalyzed C-H insertion reaction of quinoid carbene. <i>Organic Chemistry Frontiers</i> , 2022, 9, 1143-1151.	2.3	2
2	Tuning the Excited State of Tetradentate Pd(II) and Pt(II) Complexes through Benzannulated N-Heteroaromatic Ring and Central Metal. <i>Chinese Journal of Chemistry</i> , 2022, 40, 223-234.	2.6	8
3	Ni-Catalyzed Ligand-Controlled Selective 5-Exo and 6-Endo Cyclization/Cross-Couplings Involving an Unusual 1,2-Aryl Migration. <i>ACS Catalysis</i> , 2022, 12, 4131-4140.	5.5	7
4	Directed evolution of nonheme iron enzymes to access abiological radical-relay C(sp ³)-H azidation. <i>Science</i> , 2022, 376, 869-874.	6.0	36
5	Tandem 1,6-addition/cyclopropanation/rearrangement reaction of vinylogous <i>para</i> -quinone methides with 3-chlorooxindoles: construction of vicinal quaternary carbon centers. <i>Organic Chemistry Frontiers</i> , 2022, 9, 3697-3708.	2.3	3
6	Computational Exploration of Dinuclear MgCo Complex-Catalyzed Ring-Opening Copolymerization of Cyclohexene Oxide and CO ₂ . <i>Macromolecules</i> , 2022, 55, 5766-5774.	2.2	1
7	Fused 6/5/6 Metallocycle-Based Tetradentate Pt(II) Emitters for Efficient Green Phosphorescent OLEDs. <i>Inorganic Chemistry</i> , 2022, 61, 11218-11231.	1.9	8
8	Enantioselective Arylation of Tetrasubstituted Enamines: Access to Enantioenriched Indolenine and 1H-Indole Derivatives. <i>ACS Catalysis</i> , 2021, 11, 1827-1832.	5.5	11
9	<i>N</i> -Heterocyclic Carbene-Based Tetradentate Pd(II) Complexes for Deep-Blue Phosphorescent Materials. <i>Organometallics</i> , 2021, 40, 472-481.	1.1	10
10	Inherent Selectivity of Pd C-H Activation from Different Metal Oxidation States. <i>Organometallics</i> , 2021, 40, 2290-2294.	1.1	5
11	Tetradentate Platinum(II) and Palladium(II) Complexes Containing Fused 6/6/6 or 6/6/5 Metallocycles with Azacarbazolylicarbazole-Based Ligands. <i>Inorganic Chemistry</i> , 2021, 60, 12972-12983.	1.9	17
12	Rapid and highly sensitive colorimetric biosensor for the detection of glucose and hydrogen peroxide based on nanoporphyrin combined with bromine as a peroxidase-like catalyst. <i>Sensors and Actuators B: Chemical</i> , 2021, 343, 130104.	4.0	16
13	Mechanistic Investigation of Palladium-Catalyzed <i>meta</i> -C-H Bond Activation of Arenes with a Carboxyl Directing Group. <i>Journal of Organic Chemistry</i> , 2021, 86, 13475-13480.	1.7	4
14	A mechanistic study of the manganese porphyrin-catalyzed C-H isocyanation reaction. <i>Organic Chemistry Frontiers</i> , 2021, 8, 1858-1866.	2.3	7
15	N-Heterocyclic carbene-based tetradentate platinum(<i>ii</i>) complexes for phosphorescent OLEDs with high brightness. <i>Journal of Materials Chemistry C</i> , 2021, 10, 210-218.	2.7	18
16	Mechanism and stereoselectivity of benzylic C-H hydroxylation by Ru-porphyrin: a computational study. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 346-352.	1.5	8
17	Tetradentate Platinum(II) Complexes for Highly Efficient Phosphorescent Emitters and Sky Blue OLEDs. <i>Chemistry of Materials</i> , 2020, 32, 537-548.	3.2	61
18	Phosphorescent Tetradentate Platinum(II) Complexes Containing Fused 6/5/5 or 6/5/6 Metallocycles. <i>Inorganic Chemistry</i> , 2020, 59, 18109-18121.	1.9	12

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19	Computational Studies on the Mechanism and Origin of the Different Regioselectivities of Manganese Porphyrin-Catalyzed C–H Bond Hydroxylation and Amidation of Equilenin Acetate. <i>Journal of Organic Chemistry</i> , 2020, 85, 14879-14889.	1.7	17
20	Intramolecular hydrogen bond-induced high chemical stability of metal–organic frameworks. <i>Inorganic Chemistry Frontiers</i> , 2020, 7, 3548-3554.	3.0	14
21	Tuning the Excited State of Tetradentate Pd(II) Complexes for Highly Efficient Deep-Blue Phosphorescent Materials. <i>Inorganic Chemistry</i> , 2020, 59, 13502-13516.	1.9	16
22	Rh(III)-catalyzed, hydrazine-directed C–H functionalization with 1-alkynylcyclobutanols: a new strategy for 1-H-indazoles. <i>Chemical Communications</i> , 2020, 56, 7415-7418.	2.2	28
23	Highly Efficient Phosphorescent Tetradentate Platinum(II) Complexes Containing Fused 6/5/6 Metallocycles. <i>Inorganic Chemistry</i> , 2020, 59, 3718-3729.	1.9	27
24	Understanding the structures and aromaticity of heteroporphyrins with computations. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 4415-4422.	1.5	7
25	Simultaneous quantitative structure–activity relationship analysis of catalyst activity and selectivity in the direct oxidation of C–H bonds. <i>Journal of Chemometrics</i> , 2019, 33, e3165.	0.7	3
26	Computational Exploration of Chiral Iron Porphyrin-Catalyzed Asymmetric Hydroxylation of Ethylbenzene Where Stereoselectivity Arises from π – π Stacking Interaction. <i>Journal of Organic Chemistry</i> , 2019, 84, 13755-13763.	1.7	10
27	Metal-Assisted Delayed Fluorescent Pd(II) Complexes and Phosphorescent Pt(II) Complex Based on [1,2,4]Triazolo[4,3- <i>a</i>]pyridine-Containing Ligands: Synthesis, Characterization, Electrochemistry, Photophysical Studies, and Application. <i>Inorganic Chemistry</i> , 2019, 58, 14349-14360.	1.9	35
28	Highly Enantioselective Hydrogenation of Non- <i>ortho</i> -Substituted 2-Pyridyl Aryl Ketones via Iridium- <i>fac</i> -Diaphos Catalysis. <i>Organic Letters</i> , 2019, 21, 5392-5396.	2.4	30
29	Multiple roles of silver salts in palladium-catalyzed C–H activations. <i>Journal of Organometallic Chemistry</i> , 2018, 864, 19-25.	0.8	93
30	The Distortion/Interaction Model for Analysis of Activation Energies of Organic Reactions. , 2018, , 371-402.		3
31	A Highly Enantioselective Copper/Phosphoramidite–Thioether–Catalyzed Diastereodivergent 1,3-Dipolar Cycloaddition of Azomethine Ylides and Nitroalkenes. <i>Chemistry - A European Journal</i> , 2018, 24, 1714-1719.	1.7	31
32	Computational Exploration of a Pd(II)-Catalyzed β -C–H Arylation Where Stereoselectivity Arises from Attractive Aryl–Aryl Interactions. <i>Journal of Organic Chemistry</i> , 2018, 83, 14786-14790.	1.7	8
33	Computational exploration of Pd-catalyzed C–H bond activation reactions. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25723.	1.0	11
34	Design of catalysts for site-selective and enantioselective functionalization of non-activated primary C–H bonds. <i>Nature Chemistry</i> , 2018, 10, 1048-1055.	6.6	131
35	A potassium tert-butoxide and hydrosilane system for ultra-deep desulfurization of fuels. <i>Nature Energy</i> , 2017, 2, .	19.8	55
36	Potassium <i>tert</i> -Butoxide-Catalyzed Dehydrogenative C–H Silylation of Heteroaromatics: A Combined Experimental and Computational Mechanistic Study. <i>Journal of the American Chemical Society</i> , 2017, 139, 6867-6879.	6.6	160

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37	Mechanism, Regio-, and Diastereoselectivity of Rh(III)-Catalyzed Cyclization Reactions of <i>N</i> -Arylnitrones with Alkynes: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4496-4504.	1.1	17
38	Ionic and Neutral Mechanisms for C-H Bond Silylation of Aromatic Heterocycles Catalyzed by Potassium <i>tert</i> -Butoxide. <i>Journal of the American Chemical Society</i> , 2017, 139, 6880-6887.	6.6	111
39	Cage-Walking: Vertex Differentiation by Palladium-Catalyzed Isomerization of B(9)-Bromo- <i>meta</i> -Carborane. <i>Journal of the American Chemical Society</i> , 2017, 139, 7729-7732.	6.6	97
40	The Origins of Dramatic Differences in Five-Membered vs Six-Membered Chelation of Pd(II) on Efficiency of C(sp ³)-H Bond Activation. <i>Journal of the American Chemical Society</i> , 2017, 139, 8514-8521.	6.6	96
41	Palladium-Catalyzed Suzuki-Miyaura Coupling of Aryl Esters. <i>Journal of the American Chemical Society</i> , 2017, 139, 1311-1318.	6.6	212
42	Dynamic Ligand Exchange as a Mechanistic Probe in Pd-Catalyzed Enantioselective C-H Functionalization Reactions Using Monoprotected Amino Acid Ligands. <i>Journal of the American Chemical Society</i> , 2017, 139, 18500-18503.	6.6	18
43	Computational Exploration of Concerted and Zwitterionic Mechanisms of Diels-Alder Reactions between 1,2,3-Triazines and Enamines and Acceleration by Hydrogen-Bonding Solvents. <i>Journal of the American Chemical Society</i> , 2017, 139, 18213-18221.	6.6	35
44	Experimental-Computational Synergy for Selective Pd(II)-Catalyzed C-H Activation of Aryl and Alkyl Groups. <i>Accounts of Chemical Research</i> , 2017, 50, 2853-2860.	7.6	189
45	Nickel-Catalyzed Activation of Acyl C=O Bonds of Methyl Esters. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 2810-2814.	7.2	142
46	Metal-Free Synthesis of 3-Arylquinolin-2-ones from Acrylic Amides via a Highly Regioselective 1,2-Aryl Migration: An Experimental and Computational Study. <i>Journal of Organic Chemistry</i> , 2016, 81, 4058-4065.	1.7	35
47	Computational Exploration of Rh ^{III} /Rh ^V and Rh ^{III} /Rh ^I Catalysis in Rhodium(III)-Catalyzed C-H Activation Reactions of <i>N</i> -Phenoxyacetamides with Alkynes. <i>Journal of the American Chemical Society</i> , 2016, 138, 6861-6868.	6.6	116
48	Ligand-accelerated enantioselective methylene C(sp ³)-H bond activation. <i>Science</i> , 2016, 353, 1023-1027.	6.0	296
49	Nickel-Catalyzed Activation of Acyl C=O Bonds of Methyl Esters. <i>Angewandte Chemie</i> , 2016, 128, 2860-2864.	1.6	36
50	Diels-Alder Reactivities of Benzene, Pyridine, and Di-, Tri-, and Tetrazines: The Roles of Geometrical Distortions and Orbital Interactions. <i>Journal of the American Chemical Society</i> , 2016, 138, 1660-1667.	6.6	91
51	Conversion of amides to esters by the nickel-catalysed activation of amide C-N bonds. <i>Nature</i> , 2015, 524, 79-83.	13.7	479
52	Enzymatic hydroxylation of an unactivated methylene C-H bond guided by molecular dynamics simulations. <i>Nature Chemistry</i> , 2015, 7, 653-660.	6.6	100
53	Generation and Regioselective Trapping of a 3,4-Piperidyne for the Synthesis of Functionalized Heterocycles. <i>Journal of the American Chemical Society</i> , 2015, 137, 4082-4085.	6.6	64
54	Computational Exploration of Mechanism and Selectivities of (NHC)Nickel(II)hydride-Catalyzed Hydroalkenylations of Styrene with β -Olefins. <i>ACS Catalysis</i> , 2015, 5, 5545-5555.	5.5	50

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55	Ligand-Controlled Diastereoselective 1,3-Dipolar Cycloadditions of Azomethine Ylides with Methacrylonitrile. <i>Organic Letters</i> , 2015, 17, 6166-6169.	2.4	16
56	Palladium-Catalyzed <i>meta</i> -Selective C-H Bond Activation with a Nitrile-Containing Template: Computational Study on Mechanism and Origins of Selectivity. <i>Journal of the American Chemical Society</i> , 2014, 136, 344-355.	6.6	317
57	Mechanism and Selectivity of <i>N</i> -Triflylphosphoramidate Catalyzed (3 ⁺ + 2) Cycloaddition between Hydrazones and Alkenes. <i>Journal of the American Chemical Society</i> , 2014, 136, 13769-13780.	6.6	72
58	Palladium-catalyzed benzo[d]isoxazole synthesis by C-H activation/[4 + 1] annulation. <i>Chemical Science</i> , 2014, 5, 1574-1578.	3.7	67
59	Synthesis of Indolo[2,1- <i>a</i>]isoquinolines via a Triazene-Directed C-H Annulation Cascade. <i>Journal of Organic Chemistry</i> , 2014, 79, 11863-11872.	1.7	87
60	Ligand-Controlled Reactivity, Selectivity, and Mechanism of Cationic Ruthenium-Catalyzed Hydrosilylations of Alkynes, Ketones, and Nitriles: A Theoretical Study. <i>Journal of Organic Chemistry</i> , 2014, 79, 8856-8864.	1.7	44
61	Role of <i>N</i> -Acyl Amino Acid Ligands in Pd(II)-Catalyzed Remote C-H Activation of Tethered Arenes. <i>Journal of the American Chemical Society</i> , 2014, 136, 894-897.	6.6	263
62	Computational Studies on the Mechanism of the Copper-Catalyzed sp ³ -C-H Cross-Dehydrogenative Coupling Reaction. <i>ChemPlusChem</i> , 2013, 78, 943-951.	1.3	42
63	Silicon-Containing Formal 4i-Electron Four-Membered Ring Systems: Antiaromatic, Aromatic, or Nonaromatic?. <i>Chemistry - A European Journal</i> , 2012, 18, 7516-7524.	1.7	51
64	Theoretical studies on the mechanism and stereoselectivity of Rh(Phebox)-catalyzed asymmetric reductive aldol reaction. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 5845.	1.5	26
65	An Unprecedented Silver Salt Effect Switches the Facial Selectivity in the Vinylogous Mukaiyama Aldol Reaction. <i>Advanced Synthesis and Catalysis</i> , 2010, 352, 2387-2393.	2.1	11
66	Construction of All-Carbon Quaternary Center by R ₂ AlCl ⁺ -Mediated Ring-Opening Reaction of Oxacycles. <i>Organic Letters</i> , 2010, 12, 488-491.	2.4	16