

Yang Wang

List of Publications by Year in descending order

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61
papers

1,926
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172443

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#	ARTICLE	IF	CITATIONS
1	Organocatalytic insertion into C=C bonds by <i>in situ</i> generated carbene: mechanism, role of the catalyst, and origin of stereoselectivity. <i>Catalysis Science and Technology</i> , 2022, 12, 947-953.	4.1	18
2	Unraveling the mechanism and substituent effects on the N-heterocyclic carbene-catalyzed transformation reaction of enals and imines. <i>Molecular Catalysis</i> , 2022, 519, 112122.	2.0	8
3	Mechanism of a cobalt-catalyzed hydroarylation reaction and origin of stereoselectivity. <i>Catalysis Science and Technology</i> , 2022, 12, 4380-4387.	4.1	11
4	Theoretical investigation on cobalt-catalyzed hydroacylation reaction: Mechanism and origin of stereoselectivity. <i>Molecular Catalysis</i> , 2022, 527, 112410.	2.0	7
5	Insight into the organocatalytic arylation of azonaphthalenes with α -chloroaldehydes: the general mechanism and origin of selectivities. <i>Chemical Communications</i> , 2021, 57, 219-222.	4.1	29
6	Predicting the origin of selectivity in NHC-catalyzed ring opening of formylcyclopropane: a theoretical investigation. <i>Catalysis Science and Technology</i> , 2021, 11, 332-337.	4.1	28
7	Theoretical study of the NHC-catalyzed C=S bond cleavage and reconstruction reaction: mechanism, stereoselectivity, and role of catalysts. <i>Organic Chemistry Frontiers</i> , 2021, 8, 5352-5360.	4.5	16
8	Insights into the chiral sulfide/selenide-catalyzed electrophilic carbothiolation of alkynes: mechanism and origin of axial chirality. <i>Organic Chemistry Frontiers</i> , 2021, 8, 1983-1990.	4.5	20
9	Multiple Functional Organocatalyst-Promoted Inert C=C Activation: Mechanism and Origin of Selectivities. <i>ACS Catalysis</i> , 2021, 11, 3443-3454.	11.2	38
10	Mechanism and origin of diastereoselectivity of N-heterocyclic carbene-catalyzed cross-benzoin reaction: A DFT study. <i>Chinese Chemical Letters</i> , 2020, 31, 736-738.	9.0	34
11	A combined experimental and computational study of NHC-promoted desulfonylation of tosylated aldimines. <i>Organic Chemistry Frontiers</i> , 2020, 7, 578-583.	4.5	16
12	Origin of Regio- and Stereoselectivity in the NHC-catalyzed Reaction of Alkyl Pyridinium with Aliphatic Enal. <i>ChemCatChem</i> , 2020, 12, 1068-1074.	3.7	27
13	Computational Study on N-Heterocyclic Carbene (NHC)-Catalyzed Intramolecular Hydroacylation-Stetter Reaction Cascade. <i>Molecular Catalysis</i> , 2020, 484, 110723.	2.0	5
14	Origin and stabilization of axial chirality in the construction of naphthyl-C2-indoles: a DFT study. <i>Organic Chemistry Frontiers</i> , 2020, 7, 3166-3173.	4.5	8
15	Origin of diastereoselectivity and catalytic efficiency on Isothiourea-mediated cyclization of carboxylic acid with alkenyl ketone. <i>Computational and Theoretical Chemistry</i> , 2020, 1190, 113004.	2.5	1
16	Unveiling the Chemo- and Stereoselectivities of NHC-Catalyzed Reactions of an Aliphatic Ester with Aminochalcone. <i>Journal of Organic Chemistry</i> , 2020, 85, 8437-8446.	3.2	26
17	Insights into N-heterocyclic carbene and Lewis acid cooperatively catalyzed oxidative [3 + 3] annulation reactions of α,β -unsaturated aldehyde with 1,3-dicarbonyl compounds. <i>Organic Chemistry Frontiers</i> , 2020, 7, 1113-1121.	4.5	25
18	Mechanistic investigation of N-heterocyclic carbene and Na ₂ CO ₃ cooperatively catalyzed C(sp ³)-F bond activation reaction of fluoroenal. <i>Molecular Catalysis</i> , 2020, 489, 110944.	2.0	11

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19	Prediction on the Origin of Selectivities in Base-controlled Switchable NHC-catalyzed Transformations. <i>Chemistry - an Asian Journal</i> , 2019, 14, 293-300.	3.3	42
20	Mechanism and Substituent Effects of Benzene Arylation via a Phenyl Cation Strategy: A Density Functional Theory Study. <i>ChemCatChem</i> , 2019, 11, 5068-5076.	3.7	5
21	Mechanistic studies on the N-heterocyclic carbene-catalyzed reaction of isatin-derived enals with hydrazones. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 7442-7447.	2.8	25
22	Prediction on the origin of selectivities of NHC-catalyzed asymmetric dearomatization (CADA) reactions. <i>Catalysis Science and Technology</i> , 2019, 9, 465-476.	4.1	50
23	Prediction on the origin of chemoselectivity in Lewis base-mediated competition cyclizations between allenates and chalcones: a computational study. <i>Organic Chemistry Frontiers</i> , 2019, 6, 2692-2700.	4.5	23
24	Unravelling the Mechanism and Selectivity of the NHC-catalyzed Three-Membered Ring-Opening/Fluorination of Epoxy Enals: A DFT Study. <i>ChemCatChem</i> , 2019, 11, 2919-2925.	3.7	20
25	Fluorination of benzene with disubstituted N-fluoropyridinium salts in acetonitrile solution: a DFT study. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	1.4	3
26	Insights into NHC-catalyzed oxidative $\hat{I}^3\text{-C}(\text{sp}^3)\text{-H}$ activation of aliphatic aldehydes and cascade [2 + 3] cycloaddition with azomethine imines. <i>Catalysis Science and Technology</i> , 2019, 9, 2514-2522.	4.1	48
27	NHC-Catalyzed Aldol-Like Reactions of Allenates with Isatins: Regiospecific Syntheses of \hat{I}^3 -Functionalized Allenates. <i>Organic Letters</i> , 2019, 21, 1306-1310.	4.6	42
28	Insights into the isothioureia-catalyzed asymmetric [4 + 2] annulation of phenylacetic acid with alkylidene pyrazolone. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 2301-2311.	2.8	31
29	Insights into the N-Heterocyclic Carbene (NHC)-Catalyzed Intramolecular Cyclization of Aldimines: General Mechanism and Role of Catalyst. <i>Chemistry - an Asian Journal</i> , 2018, 13, 1710-1718.	3.3	34
30	Recent Advances on Computational Investigations of N-Heterocyclic Carbene Catalyzed Cycloaddition/Annulation Reactions: Mechanism and Origin of Selectivities. <i>ChemCatChem</i> , 2018, 10, 338-360.	3.7	106
31	Theoretical study on DABCO-catalyzed ring expansion of cyclopropyl ketone: Mechanism, chemoselectivity, and role of catalyst. <i>Computational and Theoretical Chemistry</i> , 2018, 1123, 20-25.	2.5	12
32	Rhodium(III)-Catalyzed Cascade [5 + 1] Annulation/5-exo-Cyclization Initiated by C-H Activation: 1,6-Diynes as One-Carbon Reaction Partners. <i>Organic Letters</i> , 2018, 20, 3245-3249.	4.6	39
33	Insights into the NHC-catalyzed cascade Michael/aldol/lactamization reaction: mechanism and origin of stereoselectivity. <i>Organic Chemistry Frontiers</i> , 2018, 5, 2065-2072.	4.5	35
34	Insights into the N-Heterocyclic Carbene (NHC)-Catalyzed Oxidative $\hat{I}^3\text{-C}(\text{sp}^3)\text{-H}$ Deprotonation of Alkylenals and Cascade [4 + 2] Cycloaddition with Alkenylisoxazoles. <i>Journal of Organic Chemistry</i> , 2018, 83, 8543-8555.	3.2	61
35	Competing mechanisms and origins of chemo- and stereo-selectivities of NHC-catalyzed reactions of enals with 2-aminoacrylates. <i>Catalysis Science and Technology</i> , 2018, 8, 4229-4240.	4.1	40
36	High-Valent Cobalt-Catalyzed C-H Activation/Annulation of 2-Benzamidopyridine 1-Oxide with Terminal Alkyne: A Combined Theoretical and Experimental Study. <i>Advanced Synthesis and Catalysis</i> , 2018, 360, 2668-2677.	4.3	61

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37	Insights into N-heterocyclic carbene-catalyzed [3 + 4] annulation reactions of 2-bromoaldehydes with N-Ts hydrazones. <i>Organic Chemistry Frontiers</i> , 2018, 5, 2739-2748.	4.5	49
38	Theoretical investigation toward organophosphine-catalyzed [3+3] annulation of Morita-Baylis-Hillman carbonates with azomethine imines: Mechanism, origin of stereoselectivity, and role of catalyst. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25367.	2.0	18
39	A DFT Study on Mechanisms and Origin of Selectivity of Phosphine-Catalyzed Vicinal Acylcyanation of Alkynoates. <i>ChemistrySelect</i> , 2017, 2, 5266-5273.	1.5	19
40	Insights into chemoselective fluorination reaction of alkynals via N-heterocyclic carbene and Brønsted base cooperative catalysis. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	1.4	11
41	Computational Study on \hat{I}^3 -C-H Functionalization of \hat{I}^1, \hat{I}^2 -Unsaturated Ester Catalyzed by N-Heterocyclic Carbene: Mechanisms, Origin of Stereoselectivity, and Role of Catalyst. <i>Journal of Organic Chemistry</i> , 2017, 82, 13043-13050.	3.2	55
42	Computational study on NHC-catalyzed enantioselective and chemoselective fluorination of aliphatic aldehydes. <i>Organic Chemistry Frontiers</i> , 2017, 4, 1987-1998.	4.5	47
43	A computational study on the N-heterocyclic carbene-catalyzed $C_{sp^2} \rightarrow C_{sp^3}$ bond activation/[4+2] cycloaddition cascade reaction of cyclobutenones with imines: a new application of the conservation principle of molecular orbital symmetry. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 19933-19943.	2.8	36
44	Insights into N-Heterocyclic Carbene-Catalyzed [4+2] Annulation Reaction of Enals with Nitroalkenes: Mechanisms, Origin of Chemo- and Stereoselectivity, and Role of Catalyst. <i>Chemistry - an Asian Journal</i> , 2016, 11, 3046-3054.	3.3	32
45	Theoretical investigations towards the [4+2] cycloaddition of ketenes with 1-azadienes catalyzed by N-heterocyclic carbenes: mechanism and stereoselectivity. <i>Tetrahedron</i> , 2016, 72, 5295-5300.	1.9	16
46	Insights into Stereoselective Aminomethylation Reaction of \hat{I}^1, \hat{I}^2 -Unsaturated Aldehyde with N,O-Acetal via N-Heterocyclic Carbene and Brønsted Acid/Base Cooperative Organocatalysis. <i>Journal of Organic Chemistry</i> , 2016, 81, 5370-5380.	3.2	59
47	A DFT study on NHC-catalyzed intramolecular aldehyde-ketone crossed-benzoin reaction: mechanism, regioselectivity, stereoselectivity, and role of NHC. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 6577-6590.	2.8	38
48	DFT Study on the Mechanism and Stereoselectivity of NHC-Catalyzed Synthesis of Substituted Trifluoromethyl Dihydropyranones with Contiguous Stereocenters. <i>Journal of Organic Chemistry</i> , 2016, 81, 868-877.	3.2	28
49	DFT perspective toward [3 + 2] annulation reaction of enals with \hat{I}^1 -ketoamides through NHC and Brønsted acid cooperative catalysis: mechanism, stereoselectivity, and role of NHC. <i>Organic Chemistry Frontiers</i> , 2016, 3, 190-203.	4.5	74
50	N-Heterocyclic Carbene (NHC)-Catalyzed $sp^3 \rightarrow sp^2$ -C-H Activation of Saturated Carbonyl Compounds: Mechanism, Role of NHC, and Origin of Stereoselectivity. <i>ACS Catalysis</i> , 2016, 6, 279-289.	11.2	99
51	A DFT study on PBu ₃ -catalyzed intramolecular cyclizations of N-allylic substituted \hat{I}^1 -amino nitriles for the formation of functionalized pyrrolidines: mechanisms, selectivities, and the role of catalysts. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 3130-3141.	2.8	32
52	Mechanisms and stereoselectivities of the Rh(<i>i</i>)-catalyzed carbenoid carbon insertion reaction of benzocyclobutenol with diazoester. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 6587-6597.	2.8	36
53	Theoretical Investigations toward the Asymmetric Insertion Reaction of Diazoester with Aldehyde Catalyzed by N-Protonated Chiral Oxazaborolidine: Mechanisms and Stereoselectivity. <i>Journal of Physical Chemistry A</i> , 2015, 119, 8422-8431.	2.5	25
54	A quantum mechanical study of the mechanism and stereoselectivity of the N-heterocyclic carbene catalyzed [4 + 2] annulation reaction of enals with azodicarboxylates. <i>Organic Chemistry Frontiers</i> , 2015, 2, 874-884.	4.5	48

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55	A DFT study on the competing mechanisms of PPh ₃ -catalyzed [3+3] and [3+2] annulations between 5-acetoxypenta-2,3-dienoate and 1C,3O-bisnucleophiles. <i>Journal of Molecular Catalysis A</i> , 2015, 407, 137-146.	4.8	18
56	Mechanistic and stereoselectivity study for the reaction of trifluoropyruvates with arylpropenes catalyzed by a cationic Lewis acid rhodium complex. <i>RSC Advances</i> , 2015, 5, 100147-100158.	3.6	15
57	DFT study on the reaction mechanisms and stereoselectivities of NHC-catalyzed [2 + 2] cycloaddition between arylalkylketenes and electron-deficient benzaldehydes. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 6374.	2.8	36
58	Mechanistic insights into the stereoselective C2-functionalization of 1-substituted imidazoles with cyanophenylacetylene and aldehydes. <i>Computational and Theoretical Chemistry</i> , 2014, 1049, 35-41.	2.5	5
59	DFT Study on the Mechanisms and Stereoselectivities of the [4 + 2] Cycloadditions of Enals and Chalcones Catalyzed by N-Heterocyclic Carbene. <i>Journal of Organic Chemistry</i> , 2014, 79, 3069-3078.	3.2	52
60	A theoretical study on the mechanisms of the reactions between 1,3-dialkynes and ammonia derivatives for the formation of five-membered N-heterocycles. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 7503-7514.	2.8	27
61	DFT Study on the Mechanisms and Diastereoselectivities of Lewis Acid-Promoted Ketene-Alkene [2 + 2] Cycloadditions: What is the Role of Lewis Acid in the Ketene and C = X (X = O, CH ₂ , and NH) [2 + 2] Cycloaddition Reactions?. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4288-4300.	2.5	46