

Lung-Wa Chung

List of Publications by Year in descending order

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85
papers

5,426
citations

76326

40
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82547

72
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96
all docs

96
docs citations

96
times ranked

6038
citing authors

#	ARTICLE	IF	CITATIONS
1	The ONIOM Method and Its Applications. <i>Chemical Reviews</i> , 2015, 115, 5678-5796.	47.7	936
2	Mechanistic Studies on the Reversible Hydrogenation of Carbon Dioxide Catalyzed by an Ir-PNP Complex. <i>Organometallics</i> , 2011, 30, 6742-6750.	2.3	288
3	Computational Organic Chemistry: Bridging Theory and Experiment in Establishing the Mechanisms of Chemical Reactions. <i>Journal of the American Chemical Society</i> , 2015, 137, 1706-1725.	13.7	271
4	The ONIOM method: its foundation and applications to metalloenzymes and photobiology. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2012, 2, 327-350.	14.6	173
5	A Theoretical Study on the Mechanism, Regiochemistry, and Stereochemistry of Hydrosilylation Catalyzed by Cationic Ruthenium Complexes. <i>Journal of the American Chemical Society</i> , 2003, 125, 11578-11582.	13.7	156
6	Novel Molecular Doping Mechanism for n-Doping of SnO ₂ via Triphenylphosphine Oxide and Its Effect on Perovskite Solar Cells. <i>Advanced Materials</i> , 2019, 31, e1805944.	21.0	152
7	Mechanistic Studies on the Formation of Linear Polyethylene Chain Catalyzed by Palladium Phosphine-Sulfonate Complexes: Experiment and Theoretical Studies. <i>Journal of the American Chemical Society</i> , 2009, 131, 14088-14100.	13.7	146
8	Ligand-Controlled Remarkable Regio- and Stereodivergence in Intermolecular Hydrosilylation of Internal Alkynes: Experimental and Theoretical Studies. <i>Journal of the American Chemical Society</i> , 2013, 135, 13835-13842.	13.7	135
9	Organocatalytic atroposelective synthesis of axially chiral styrenes. <i>Nature Communications</i> , 2017, 8, 15238.	12.8	128
10	New Mechanistic Insights on the Selectivity of Transition-Metal-Catalyzed Organic Reactions: The Role of Computational Chemistry. <i>Accounts of Chemical Research</i> , 2016, 49, 1302-1310.	15.6	100
11	Highly efficient and practical resolution of 1,1-spirobiindane-7,7-diol by inclusion crystallization with N-benzylcinchonidinium chloride. <i>Tetrahedron: Asymmetry</i> , 2002, 13, 1363-1366.	1.8	91
12	Mechanism of Efficient Firefly Bioluminescence via Adiabatic Transition State and Seam of Sloped Conical Intersection. <i>Journal of the American Chemical Society</i> , 2008, 130, 12880-12881.	13.7	88
13	Nickel-catalyzed asymmetric hydrogenation of $\hat{1}^2$ -acylamino nitroolefins: an efficient approach to chiral amines. <i>Chemical Science</i> , 2017, 8, 6419-6422.	7.4	82
14	Computational Study on the Reaction Mechanism of Hydrosilylation of Carbonyls Catalyzed by High-Valent Rhenium(V)-Di-oxo Complexes. <i>Journal of Organic Chemistry</i> , 2006, 71, 6000-6009.	3.2	81
15	Density Functional Theory Study on a Missing Piece in Understanding of Heme Chemistry: The Reaction Mechanism for Indoleamine 2,3-Dioxygenase and Tryptophan 2,3-Dioxygenase. <i>Journal of the American Chemical Society</i> , 2008, 130, 12299-12309.	13.7	80
16	Iridium-Catalyzed Asymmetric Hydrogenation of Ketones with Accessible and Modular Ferrocene-Based Amino-phosphine Acid (f-Ampha) Ligands. <i>Organic Letters</i> , 2017, 19, 690-693.	4.6	79
17	Why Did Incorporation of Acrylonitrile to a Linear Polyethylene Become Possible? Comparison of Phosphine-Sulfonate Ligand with Diphosphine and Imine-Phenolate Ligands in the Pd-Catalyzed Ethylene/Acrylonitrile Copolymerization. <i>Journal of the American Chemical Society</i> , 2010, 132, 16030-16042.	13.7	78
18	Dearomative Indole [5+2] Cycloaddition Reactions: Stereoselective Synthesis of Highly Functionalized Cyclohepta[<i>b</i>]indoles. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 11051-11055.	13.8	77

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19	Highly Regio- and Stereoselective Hydrosilylation of Internal Thioalkynes under Mild Conditions. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 5632-5635.	13.8	77
20	Mechanism of Ni-NHC Catalyzed Hydrogenolysis of Aryl Ethers: Roles of the Excess Base. <i>ACS Catalysis</i> , 2016, 6, 483-493.	11.2	76
21	Elucidating the Key Role of Phosphine-Sulfonate Ligands in Palladium-Catalyzed Ethylene Polymerization: Effect of Ligand Structure on the Molecular Weight and Linearity of Polyethylene. <i>ACS Catalysis</i> , 2016, 6, 6101-6113.	11.2	75
22	ONIOM Study on a Missing Piece in Our Understanding of Heme Chemistry: Bacterial Tryptophan 2,3-Dioxygenase with Dual Oxidants. <i>Journal of the American Chemical Society</i> , 2010, 132, 11993-12005.	13.7	74
23	Efficient syntheses of (â)-crinine and (â)-aspidospermidine, and the formal synthesis of (â)-minfiensine by enantioselective intramolecular dearomative cyclization. <i>Chemical Science</i> , 2017, 8, 6247-6256.	7.4	71
24	A Theoretical Study on the Nature of On- and Off-States of Reversibly Photoswitching Fluorescent Protein Dronpa: Absorption, Emission, Protonation, and Raman. <i>Journal of Physical Chemistry B</i> , 2010, 114, 1114-1126.	2.6	69
25	Design and Application of Hybrid Phosphorus Ligands for Enantioselective Rh-Catalyzed Anti-Markovnikov Hydroformylation of Unfunctionalized 1,1-Disubstituted Alkenes. <i>Journal of the American Chemical Society</i> , 2018, 140, 4977-4981.	13.7	64
26	Pd-Catalyzed Copolymerization of Methyl Acrylate with Carbon Monoxide: Structures, Properties and Mechanistic Aspects toward Ligand Design. <i>Journal of the American Chemical Society</i> , 2011, 133, 6761-6779.	13.7	63
27	Brønsted-Acid-Promoted Rh-Catalyzed Asymmetric Hydrogenation of N-Unprotected Indoles: A Cocatalysis of Transition Metal and Anion Binding. <i>Organic Letters</i> , 2018, 20, 2143-2147.	4.6	62
28	Regiospecific and Enantioselective Arylvinylcarbene Insertion of a C-H Bond of Aniline Derivatives Enabled by a Rh(I)-Diene Catalyst. <i>Journal of the American Chemical Society</i> , 2021, 143, 2608-2619.	13.7	61
29	Enzyme-Inspired Chiral Secondary-Phosphine-Oxide Ligand with Dual Noncovalent Interactions for Asymmetric Hydrogenation. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 6808-6812.	13.8	60
30	Ferrocenyl chiral bisphosphorus ligands for highly enantioselective asymmetric hydrogenation via noncovalent ion pair interaction. <i>Chemical Science</i> , 2016, 7, 6669-6673.	7.4	60
31	Enantioselective Hydrogenation of Tetrasubstituted $\hat{1},\hat{1}$ -Unsaturated Carboxylic Acids Enabled by Cobalt(II) Catalysis: Scope and Mechanistic Insights. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 11384-11390.	13.8	58
32	A Combined DFT/IM-MS Study on the Reaction Mechanism of Cationic Ru(II)-Catalyzed Hydroboration of Alkynes. <i>ACS Catalysis</i> , 2017, 7, 1361-1368.	11.2	56
33	Practical and Asymmetric Reductive Coupling of Isoquinolines Templated by Chiral Diborons. <i>Journal of the American Chemical Society</i> , 2017, 139, 9767-9770.	13.7	54
34	Experimental and Theoretical Studies of the Propargyl-Allenylindium System. <i>Journal of the American Chemical Society</i> , 2004, 126, 13326-13334.	13.7	53
35	DFT and ONIOM(DFT:MM) Studies on Co-C Bond Cleavage and Hydrogen Transfer in B_{12} -Dependent Methylmalonyl-CoA Mutase. Stepwise or Concerted Mechanism?. <i>Journal of the American Chemical Society</i> , 2009, 131, 5115-5125.	13.7	53
36	Comparative Reactivity of Ferric-Superoxo and Ferryl-Oxo Species in Heme and Non-Heme Complexes. <i>Journal of the American Chemical Society</i> , 2011, 133, 20076-20079.	13.7	52

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37	Primary Events of Photodynamics in Reversible Photoswitching Fluorescent Protein Dronpa. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 3328-3333.	4.6	51
38	Enantioselective palladium-catalyzed diboration of 1,1-disubstituted allenes. <i>Chemical Science</i> , 2017, 8, 5161-5165.	7.4	51
39	Ru-Catalyzed Geminal Hydroboration of Silyl Alkynes via a New <i>gem</i> -Addition Mechanism. <i>Journal of the American Chemical Society</i> , 2020, 142, 13867-13877.	13.7	46
40	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.	3.2	44
41	Hydrogenation of Aldehydes Catalyzed by an Available Ruthenium Complex. <i>Organic Letters</i> , 2016, 18, 1518-1521.	4.6	39
42	Reaction Mechanism of Cu(I)-Mediated Reductive CO ₂ Coupling for the Selective Formation of Oxalate: Cooperative CO ₂ Reduction To Give Mixed-Valence Cu ₂ (CO ₂) ⁺ and Nucleophilic-Like Attack. <i>Inorganic Chemistry</i> , 2017, 56, 6809-6819.	4.0	39
43	Ru-Catalyzed Migratory Geminal Semihydrogenation of Internal Alkynes to Terminal Olefins. <i>Journal of the American Chemical Society</i> , 2019, 141, 17441-17451.	13.7	38
44	Competitive Mechanistic Pathways for Green-to-Red Photoconversion in the Fluorescent Protein Kaede: A Computational Study. <i>Journal of Physical Chemistry B</i> , 2010, 114, 16666-16675.	2.6	37
45	Rhodium-catalyzed asymmetric hydrogenation of $\hat{\nu}^2$ -cyanocinnamic esters with the assistance of a single hydrogen bond in a precise position. <i>Chemical Science</i> , 2018, 9, 1919-1924.	7.4	35
46	$\hat{\nu}^2$ -Substituted Alkenyl Heteroarenes as Dipolarophiles in the Cu(I)-Catalyzed Asymmetric 1,3-Dipolar Cycloaddition of Azomethine Ylides Empowered by a Dual Activation Strategy: Stereoselectivity and Mechanistic Insight. <i>Journal of the American Chemical Society</i> , 2021, 143, 3519-3535.	13.7	34
47	A DFT Study on the Mechanism of Hydrosilylation of Unsaturated Compounds with Neutral Hydrido(hydrosilylene)tungsten Complex. <i>Journal of Organic Chemistry</i> , 2008, 73, 820-829.	3.2	33
48	Catalytic asymmetric trifluoromethylthiolation of carbonyl compounds <i>via</i> a diastereo and enantioselective Cu-catalyzed tandem reaction. <i>Chemical Communications</i> , 2018, 54, 4581-4584.	4.1	33
49	Photodynamics of All- <i>trans</i> Retinal Protonated Schiff Base in Bacteriorhodopsin and Methanol Solution. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2694-2698.	5.3	30
50	Asymmetric Total Synthesis of Cerorubenic Acid-III. <i>Journal of the American Chemical Society</i> , 2019, 141, 2872-2877.	13.7	30
51	Unusual KIE and dynamics effects in the Fe-catalyzed hetero-Diels-Alder reaction of unactivated aldehydes and dienes. <i>Nature Communications</i> , 2020, 11, 1850.	12.8	30
52	Reaction Mechanism of Photoinduced Decarboxylation of the Photoactivatable Green Fluorescent Protein: An ONIOM(QM:MM) Study. <i>Journal of Physical Chemistry B</i> , 2013, 117, 1075-1084.	2.6	29
53	Alternative Mechanistic Strategy for Enzyme Catalysis in a Ni-Dependent Lactate Racemase (LarA): Intermediate Destabilization by the Cofactor. <i>Chemistry - A European Journal</i> , 2017, 23, 3623-3630.	3.3	28
54	Silicon-oriented regio- and enantioselective rhodium-catalyzed hydroformylation. <i>Nature Communications</i> , 2018, 9, 2045.	12.8	28

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55	A Theoretical Study on the <i>trans</i> -Addition Intramolecular Hydroacylation of 4-Alkynals Catalyzed by Cationic Rhodium Complexes. <i>Journal of Organic Chemistry</i> , 2008, 73, 2649-2655.	3.2	27
56	Computational Prediction of Excited-State Carbon Tunneling in the Two Steps of Triplet Zimmerman Di- β -Methane Rearrangement. <i>Journal of the American Chemical Society</i> , 2017, 139, 16438-16441.	13.7	26
57	Kinetic Resolution of Alkylidene Norcamphors via a Ligand-Controlled Umpolung-Type 1,3-Dipolar Cycloaddition. <i>IScience</i> , 2019, 11, 146-159.	4.1	25
58	N-Bridged Pincer Iridium Complexes for Highly Efficient Alkane Dehydrogenation and the Relevant Linker Effects. <i>ACS Catalysis</i> , 2020, 10, 6475-6487.	11.2	25
59	Enzyme-Inspired Chiral Secondary-Phosphine-Oxide Ligand with Dual Noncovalent Interactions for Asymmetric Hydrogenation. <i>Angewandte Chemie</i> , 2017, 129, 6912-6916.	2.0	22
60	Asymmetric synthesis of quaternary β -trifluoromethyl β -amino acids by Ir-catalyzed allylation followed by kinetic resolution. <i>Chemical Communications</i> , 2020, 56, 3333-3336.	4.1	22
61	Theoretical Study of the Intrinsic Reactivities of Various Allylmetals toward Carbonyls and Water. <i>Organometallics</i> , 2005, 24, 1598-1607.	2.3	21
62	New Tricks for an Old Dog: Grubbs Catalysts Enable Efficient Hydrogen Production from Aqueous-Phase Methanol Reforming. <i>ACS Catalysis</i> , 2022, 12, 2212-2222.	11.2	21
63	Guest-Induced Folding and Self-Assembly of Conformationally Adaptive Macrocycles into Nanosheets and Nanotubes. <i>Chemistry - A European Journal</i> , 2017, 23, 1516-1520.	3.3	19
64	A Missing Piece of the Mechanism in Metal-Catalyzed Hydrogenation: Co(π -I)/Co(0)/Co(+I) Catalytic Cycle for Co(π -I)-Catalyzed Hydrogenation. <i>Organic Letters</i> , 2019, 21, 360-364.	4.6	19
65	Development of a novel secondary phosphine oxide-ruthenium catalyst and its application for carbonyl reduction. <i>Chemical Communications</i> , 2018, 54, 535-538.	4.1	18
66	New Insights and Predictions into Complex Homogeneous Reactions Enabled by Computational Chemistry in Synergy with Experiments: Isotopes and Mechanisms. <i>Accounts of Chemical Research</i> , 2022, 55, 1109-1123.	15.6	18
67	Theoretical Study on the UVR8 Photoreceptor: Sensing Ultraviolet-B by Tryptophan and Dissociation of Homodimer. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3319-3330.	5.3	17
68	Zinc-Homocysteine binding in cobalamin-dependent methionine synthase and its role in the substrate activation: DFT, ONIOM, and QM/MM molecular dynamics studies. <i>Journal of Computational Chemistry</i> , 2011, 32, 3154-3167.	3.3	16
69	Excited-State Proton Transfer Controls Irreversibility of Photoisomerization in Mononuclear Ruthenium(II) Monoaquo Complexes: A DFT Study. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 668-675.	5.3	16
70	Enantioselective Rhodium-Catalyzed Cycloisomerization of 1,6-Allenynes to access 5/6-Fused Bicycle[4.3.0]nonadienes. <i>Nature Communications</i> , 2019, 10, 949.	12.8	16
71	Enantioselective Hydrogenation of Tetrasubstituted β,β -Unsaturated Carboxylic Acids Enabled by Cobalt(II) Catalysis: Scope and Mechanistic Insights. <i>Angewandte Chemie</i> , 2021, 133, 11485-11491.	2.0	15
72	Exploiting the trifluoroethyl group as a precatalyst ligand in nickel-catalyzed Suzuki-type alkylations. <i>Chemical Science</i> , 2019, 10, 5275-5282.	7.4	14

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73	Mechanistic insights into asymmetric reductive coupling of isoquinolines by a chiral diboron with DFT calculations. <i>Journal of Organometallic Chemistry</i> , 2018, 864, 97-104.	1.8	13
74	Computational Insights into the Reaction Mechanisms of Nickel-Catalyzed Hydrofunctionalizations and Nickel-Dependent Enzymes. <i>Asian Journal of Organic Chemistry</i> , 2018, 7, 522-536.	2.7	12
75	Multiscale Simulations on Spectral Tuning and the Photoisomerization Mechanism in Fluorescent RNA Spinach. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5453-5464.	5.3	11
76	Rhodium(I) Carbene-Promoted Enantioselective C ^α -H Functionalization of Simple Unprotected Indoles, Pyrroles and Heteroanalogues: New Mechanistic Insights. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	11
77	Ir-Catalyzed Asymmetric Hydrogenation of Unprotected Indoles: Scope Investigations and Mechanistic Studies. <i>CCS Chemistry</i> , 2023, 5, 1398-1410.	7.8	10
78	Asymmetric Total Synthesis of Phomarol. <i>CCS Chemistry</i> , 2021, 3, 348-357.	7.8	9
79	Water as a Direct Proton Source for Asymmetric Hydroarylation Catalyzed by a Rh(I)-Diene: Access to Nonproteinogenic $\beta^2/\beta^3/\beta^2$ -Amino Acid Derivatives. <i>Organic Letters</i> , 2021, 23, 571-577.	4.6	9
80	Multiscale Quantum Refinement Approaches for Metalloproteins. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3783-3796.	5.3	8
81	A THEORETICAL STUDY ON THE INTERMOLECULAR HYDROACYLATION OF ALKYNE CATALYZED BY CATIONIC RHODIUM COMPLEX. <i>Journal of Theoretical and Computational Chemistry</i> , 2005, 04, 737-749.	1.8	7
82	Enantioselective Palladium-Catalyzed Decarboxylative Allylation of β^2 -Keto Esters Assisted by a Thiourea. <i>Synlett</i> , 2018, 29, 51-56.	1.8	7
83	Colorimetric Calcium Probe with Comparison to an Ion-Selective Optode. <i>ACS Omega</i> , 2018, 3, 12476-12481.	3.5	6
84	A Computational Study of Asymmetric Hydrogenation of α -Phenyl Acrylic Acids Catalyzed by a Rh(I) Catalyst with Ferrocenyl Chiral Bisphosphorus Ligand: The Role of Ion-Pair Interaction. <i>Chinese Journal of Chemistry</i> , 2021, 39, 1616-1624.	4.9	4
85	AgN ₃ -Catalyzed Hydroazidation of Terminal Alkynes and Mechanistic Studies. <i>Chinese Journal of Organic Chemistry</i> , 2020, 40, 2603.	1.3	0