Lung-Wa Chung

List of Publications by Year
in descending order

85	5,426	76294	82499
papers	citations	40 h-index	72 g-index

96	96	96	6038
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The ONIOM Method and Its Applications. Chemical Reviews, 2015, 115, 5678-5796.	23.0	936
2	Mechanistic Studies on the Reversible Hydrogenation of Carbon Dioxide Catalyzed by an Ir-PNP Complex. Organometallics, 2011, 30, 6742-6750.	1.1	288
3	Computational Organic Chemistry: Bridging Theory and Experiment in Establishing the Mechanisms of Chemical Reactions. Journal of the American Chemical Society, 2015, 137, 1706-1725.	6.6	271
4	The ONIOM method: its foundation and applications to metalloenzymes and photobiology. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 327-350.	6.2	173
5	A Theoretical Study on the Mechanism, Regiochemistry, and Stereochemistry of Hydrosilylation Catalyzed by Cationic Ruthenium Complexes. Journal of the American Chemical Society, 2003, 125, 11578-11582.	6.6	156
6	Novel Molecular Doping Mechanism for nâ€Doping of SnO₂ via Triphenylphosphine Oxide and Its Effect on Perovskite Solar Cells. Advanced Materials, 2019, 31, e1805944.	11.1	152
7	Mechanistic Studies on the Formation of Linear Polyethylene Chain Catalyzed by Palladium Phosphineâ^'Sulfonate Complexes: Experiment and Theoretical Studies. Journal of the American Chemical Society, 2009, 131, 14088-14100.	6.6	146
8	Ligand-Controlled Remarkable Regio- and Stereodivergence in Intermolecular Hydrosilylation of Internal Alkynes: Experimental and Theoretical Studies. Journal of the American Chemical Society, 2013, 135, 13835-13842.	6.6	135
9	Organocatalytic atroposelective synthesis of axially chiral styrenes. Nature Communications, 2017, 8, 15238.	5.8	128
10	New Mechanistic Insights on the Selectivity of Transition-Metal-Catalyzed Organic Reactions: The Role of Computational Chemistry. Accounts of Chemical Research, 2016, 49, 1302-1310.	7.6	100
11	Highly efficient and practical resolution of 1,1â€²-spirobiindane-7,7â€²-diol by inclusion crystallization with N-benzylcinchonidinium chloride. Tetrahedron: Asymmetry, 2002, 13, 1363-1366.	1.8	91
12	Mechanism of Efficient Firefly Bioluminescence via Adiabatic Transition State and Seam of Sloped Conical Intersection. Journal of the American Chemical Society, 2008, 130, 12880-12881.	6.6	88
13	Nickel-catalyzed asymmetric hydrogenation of Î²-acylamino nitroolefins: an efficient approach to chiral amines. Chemical Science, 2017, 8, 6419-6422.	3.7	82
14	Computational Study on the Reaction Mechanism of Hydrosilylation of Carbonyls Catalyzed by High-Valent Rhenium(V)â^'Di-oxo Complexes. Journal of Organic Chemistry, 2006, 71, 6000-6009.	1.7	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. Journal of the American Chemical Society, 2008, 130, 12299-12309.	6.6	80
16	Iridium-Catalyzed Asymmetric Hydrogenation of Ketones with Accessible and Modular Ferrocene-Based Amino-phosphine Acid (f-Ampha) Ligands. Organic Letters, 2017, 19, 690-693.	2.4	79
17	Why Did Incorporation of Acrylonitrile to a Linear Polyethylene Become Possible? Comparison of Phosphineâ^'Sulfonate Ligand with Diphosphine and Imineâ^'Phenolate Ligands in the Pd-Catalyzed Ethylene/Acrylonitrile Copolymerization. Journal of the American Chemical Society, 2010, 132, 16030-16042.	6.6	78
18	Dearomative Indole [5+2] Cycloaddition Reactions: Stereoselective Synthesis of Highly Functionalized Cyclohepta[b]indoles. Angewandte Chemie - International Edition, 2014, 53, 11051-11055.	7.2	77

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19	Highly Regioâ€•and Stereoselective Hydrosilylation of Internal Thioalkynes under Mild Conditions. Angewandte Chemie - International Edition, 2015, 54, 5632-5635.	7.2	77
20	Mechanism of Ni-NHC Catalyzed Hydrogenolysis of Aryl Ethers: Roles of the Excess Base. ACS Catalysis, 2016, 6, 483-493.	5.5	76
21	Elucidating the Key Role of Phosphineâ^'Sulfonate Ligands in Palladium-Catalyzed Ethylene Polymerization: Effect of Ligand Structure on the Molecular Weight and Linearity of Polyethylene. ACS Catalysis, 2016, 6, 6101-6113.	5.5	75
22	ONIOM Study on a Missing Piece in Our Understanding of Heme Chemistry: Bacterial Tryptophan 2,3-Dioxygenase with Dual Oxidants. Journal of the American Chemical Society, 2010, 132, 11993-12005.	6.6	74
23	Efficient syntheses of (â^')-crinine and (â^')-aspidospermidine, and the formal synthesis of (â^')-minfiensine by enantioselective intramolecular dearomative cyclization. Chemical Science, 2017, 8, 6247-6256.	3.7	71
24	A Theoretical Study on the Nature of On- and Off-States of Reversibly Photoswitching Fluorescent Protein Dronpa: Absorption, Emission, Protonation, and Raman. Journal of Physical Chemistry B, 2010, 114, 1114-1126.	1.2	69
25	Design and Application of Hybrid Phosphorus Ligands for Enantioselective Rh-Catalyzed Anti-Markovnikov Hydroformylation of Unfunctionalized 1,1-Disubstituted Alkenes. Journal of the American Chemical Society, 2018, 140, 4977-4981.	6.6	64
26	Pd-Catalyzed Copolymerization of Methyl Acrylate with Carbon Monoxide: Structures, Properties and Mechanistic Aspects toward Ligand Design. Journal of the American Chemical Society, 2011, 133, 6761-6779.	6.6	63
27	BrÃ¸nsted-Acid-Promoted Rh-Catalyzed Asymmetric Hydrogenation of N-Unprotected Indoles: A Cocatalysis of Transition Metal and Anion Binding. Organic Letters, 2018, 20, 2143-2147.	2.4	62
28	Regiospecific and Enantioselective Arylvinylcarbene Insertion of a Câ€“H Bond of Aniline Derivatives Enabled by a Rh(I)-Diene Catalyst. Journal of the American Chemical Society, 2021, 143, 2608-2619.	6.6	61
29	Enzymeâ€Inspired Chiral Secondaryâ€Phosphineâ€Oxide Ligand with Dual Noncovalent Interactions for Asymmetric Hydrogenation. Angewandte Chemie - International Edition, 2017, 56, 6808-6812.	7.2	60
30	Ferrocenyl chiral bisphosphorus ligands for highly enantioselective asymmetric hydrogenation via noncovalent ion pair interaction. Chemical Science, 2016, 7, 6669-6673.	3.7	60
31	Enantioselective Hydrogenation of Tetrasubstituted Î±,Î²â€Unsaturated Carboxylic Acids Enabled by Cobalt(II) Catalysis: Scope and Mechanistic Insights. Angewandte Chemie - International Edition, 2021, 60, 11384-11390.	7.2	58
32	A Combined DFT/IM-MS Study on the Reaction Mechanism of Cationic Ru(II)-Catalyzed Hydroboration of Alkynes. ACS Catalysis, 2017, 7, 1361-1368.	5.5	56
33	Practical and Asymmetric Reductive Coupling of Isoquinolines Templated by Chiral Diborons. Journal of the American Chemical Society, 2017, 139, 9767-9770.	6.6	54
34	Experimental and Theoretical Studies of the Propargyl-Allenylindium System. Journal of the American Chemical Society, 2004, 126, 13326-13334.	6.6	53
35	DFT and ONIOM(DFT:MM) Studies on Coâ^'C Bond Cleavage and Hydrogen Transfer in B₁₂-Dependent Methylmalonyl-CoA Mutase. Stepwise or Concerted Mechanism?. Journal of the American Chemical Society, 2009, 131, 5115-5125.	6.6	53
36	Comparative Reactivity of Ferric-Superoxo and Ferryl-Oxo Species in Heme and Non-Heme Complexes. Journal of the American Chemical Society, 2011, 133, 20076-20079.	6.6	52

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37	Primary Events of Photodynamics in Reversible Photoswitching Fluorescent Protein Dronpa. Journal of Physical Chemistry Letters, 2010, 1, 3328-3333.	2.1	51
38	Enantioselective palladium-catalyzed diboration of 1,1-disubstituted allenes. Chemical Science, 2017, 8, 5161-5165.	3.7	51
39	Ru-Catalyzed Geminal Hydroboration of Silyl Alkynes via a Newgem-Addition Mechanism. Journal of the American Chemical Society, 2020, 142, 13867-13877.	6.6	46
40	Ligand-Controlled Reactivity, Selectivity, and Mechanism of Cationic Ruthenium-Catalyzed Hydrosilylations of Alkynes, Ketones, and Nitriles: A Theoretical Study. Journal of Organic Chemistry, 2014, 79, 8856-8864.	1.7	44
41	Hydrogenation of Aldehydes Catalyzed by an Available Ruthenium Complex. Organic Letters, 2016, 18, 1518-1521.	2.4	39
42	Reaction Mechanism of Cu(I)-Mediated Reductive CO₂ Coupling for the Selective Formation of Oxalate: Cooperative CO₂ Reduction To Give Mixed-Valence Cu₂(CO₂^{â€¢â€“}) and Nucleophilic-Like Attack. Inorganic Chemistry, 2017, 56, 6809-6819.	1.9	39
43	Ru-Catalyzed Migratory Geminal Semihydrogenation of Internal Alkynes to Terminal Olefins. Journal of the American Chemical Society, 2019, 141, 17441-17451.	6.6	38
44	Competitive Mechanistic Pathways for Green-to-Red Photoconversion in the Fluorescent Protein Kaede: A Computational Study. Journal of Physical Chemistry B, 2010, 114, 16666-16675.	1.2	37
45	Rhodium-catalyzed asymmetric hydrogenation of Î²-cyanocinnamic esters with the assistance of a single hydrogen bond in a precise position. Chemical Science, 2018, 9, 1919-1924.	3.7	35
46	Î²-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. Journal of the American Chemical Society, 2021, 143, 3519-3535.	6.6	34
47	A DFT Study on the Mechanism of Hydrosilylation of Unsaturated Compounds with Neutral Hydrido(hydrosilylene)tungsten Complex. Journal of Organic Chemistry, 2008, 73, 820-829.	1.7	33
48	Catalytic asymmetric trifluoromethylthiolation of carbonyl compounds via a diastereo and enantioselective Cu-catalyzed tandem reaction. Chemical Communications, 2018, 54, 4581-4584.	2.2	33
49	Photodynamics of All-trans Retinal Protonated Schiff Base in Bacteriorhodopsin and Methanol Solution. Journal of Chemical Theory and Computation, 2011, 7, 2694-2698.	2.3	30
50	Asymmetric Total Synthesis of Cerorubenic Acid-III. Journal of the American Chemical Society, 2019, 141, 2872-2877.	6.6	30
51	Unusual KIE and dynamics effects in the Fe-catalyzed hetero-Diels-Alder reaction of unactivated aldehydes and dienes. Nature Communications, 2020, 11, 1850.	5.8	30
52	Reaction Mechanism of Photoinduced Decarboxylation of the Photoactivatable Green Fluorescent Protein: An ONIOM(QM:MM) Study. Journal of Physical Chemistry B, 2013, 117, 1075-1084.	1.2	29
53	Alternative Mechanistic Strategy for Enzyme Catalysis in a Niâ€Đependent Lactate Racemase (LarA): Intermediate Destabilization by the Cofactor. Chemistry - A European Journal, 2017, 23, 3623-3630.	1.7	28
54	Silicon-oriented regio- and enantioselective rhodium-catalyzed hydroformylation. Nature Communications, 2018, 9, 2045.	5.8	28

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55	A Theoretical Study on the trans-Addition Intramolecular Hydroacylation of 4-Alkynals Catalyzed by Cationic Rhodium Complexes. Journal of Organic Chemistry, 2008, 73, 2649-2655.	1.7	27
56	Computational Prediction of Excited-State Carbon Tunneling in the Two Steps of Triplet Zimmerman Di-ï€-Methane Rearrangement. Journal of the American Chemical Society, 2017, 139, 16438-16441.	6.6	26
57	Kinetic Resolution of Alkylidene Norcamphors via a Ligand-Controlled Umpolung-Type 1,3-Dipolar Cycloaddition. IScience, 2019, 11, 146-159.	1.9	25
58	N-Bridged Pincer Iridium Complexes for Highly Efficient Alkane Dehydrogenation and the Relevant Linker Effects. ACS Catalysis, 2020, 10, 6475-6487.	5.5	25
59	Enzymeâ€Inspired Chiral Secondaryâ€Phosphineâ€Oxide Ligand with Dual Noncovalent Interactions for Asymmetric Hydrogenation. Angewandte Chemie, 2017, 129, 6912-6916.	1.6	22
60	Asymmetric synthesis of quaternary Î±-trifluoromethyl Î±-amino acids by Ir-catalyzed allylation followed by kinetic resolution. Chemical Communications, 2020, 56, 3333-3336.	2.2	22
61	Theoretical Study of the Intrinsic Reactivities of Various Allylmetals toward Carbonyls and Water. Organometallics, 2005, 24, 1598-1607.	1.1	21
62	New Tricks for an Old Dog: Grubbs Catalysts Enable Efficient Hydrogen Production from Aqueous-Phase Methanol Reforming. ACS Catalysis, 2022, 12, 2212-2222.	5.5	21
63	Guestâ€Induced Folding and Selfâ€Assembly of Conformationally Adaptive Macrocycles into Nanosheets and Nanotubes. Chemistry - A European Journal, 2017, 23, 1516-1520.	1.7	19
64	A Missing Piece of the Mechanism in Metal-Catalyzed Hydrogenation: Co(â^I)/Co(0)/Co(+I) Catalytic Cycle for Co(â^I)-Catalyzed Hydrogenation. Organic Letters, 2019, 21, 360-364.	2.4	19
65	Development of a novel secondary phosphine oxideâ€“ruthenium(<scp>II</scp>) catalyst and its application for carbonyl reduction. Chemical Communications, 2018, 54, 535-538.	2.2	18
66	New Insights and Predictions into Complex Homogeneous Reactions Enabled by Computational Chemistry in Synergy with Experiments: Isotopes and Mechanisms. Accounts of Chemical Research, 2022, 55, 1109-1123.	7.6	18
67	Theoretical Study on the UVR8 Photoreceptor: Sensing Ultraviolet-B by Tryptophan and Dissociation of Homodimer. Journal of Chemical Theory and Computation, 2014, 10, 3319-3330.	2.3	17
68	Zincâ€“Homocysteine binding in cobalaminâ€dependent methionine synthase and its role in the substrate activation: DFT, ONIOM, and QM/MM molecular dynamics studies. Journal of Computational Chemistry, 2011, 32, 3154-3167.	1.5	16
69	Excited-State Proton Transfer Controls Irreversibility of Photoisomerization in Mononuclear Ruthenium(II) Monoaquo Complexes: A DFT Study. Journal of Chemical Theory and Computation, 2014, 10, 668-675.	2.3	16
70	Enantioselective Rhodium-Catalyzed Cycloisomerization of 1,6-Allenynes to access 5/6-Fused Bicycle[4.3.0]nonadienes. Nature Communications, 2019, 10, 949.	5.8	16
71	Enantioselective Hydrogenation of Tetrasubstituted Î±,Î²â€Unsaturated Carboxylic Acids Enabled by Cobalt(II) Catalysis: Scope and Mechanistic Insights. Angewandte Chemie, 2021, 133, 11485-11491.	1.6	15
72	Exploiting the trifluoroethyl group as a precatalyst ligand in nickel-catalyzed Suzuki-type alkylations. Chemical Science, 2019, 10, 5275-5282.	3.7	14

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73	Mechanistic insights into asymmetric reductive coupling of isoquinolines by a chiral diboron with DFT calculations. Journal of Organometallic Chemistry, 2018, 864, 97-104.	0.8	13
74	Computational Insights into the Reaction Mechanisms of Nickelâ€Catalyzed Hydrofunctionalizations and Nickelâ€Dependent Enzymes. Asian Journal of Organic Chemistry, 2018, 7, 522-536.	1.3	12
75	Multiscale Simulations on Spectral Tuning and the Photoisomerization Mechanism in Fluorescent RNA Spinach. Journal of Chemical Theory and Computation, 2016, 12, 5453-5464.	2.3	11
76	Rhodium(I) Carbeneâ€Promoted Enantioselective Câ^'H Functionalization of Simple Unprotected Indoles, Pyrroles and Heteroanalogues: New Mechanistic Insights. Angewandte Chemie - International Edition, 2022, 61, .	7.2	11
77	Ir-Catalyzed Asymmetric Hydrogenation of Unprotected Indoles: Scope Investigations and Mechanistic Studies. CCS Chemistry, 2023, 5, 1398-1410.	4.6	10
78	Asymmetric Total Synthesis of Phomarol. CCS Chemistry, 2021, 3, 348-357.	4.6	9
79	Water as a Direct Proton Source for Asymmetric Hydroarylation Catalyzed by a Rh(I)â€"Diene: Access to Nonproteinogenic Î²2/Î³2/Î´2-Amino Acid Derivatives. Organic Letters, 2021, 23, 571-577.	2.4	9
80	Multiscale Quantum Refinement Approaches for Metalloproteins. Journal of Chemical Theory and Computation, 2021, 17, 3783-3796.	2.3	8
81	A THEORETICAL STUDY ON THE INTERMOLECULAR HYDROACYLATION OF ALKYNE CATALYZED BY CATIONIC RHODIUM COMPLEX. Journal of Theoretical and Computational Chemistry, 2005, 04, 737-749.	1.8	7
82	Enantioselective Palladium-Catalyzed Decarboxylative Allylation of Î²-Keto Esters Assisted by a Thiourea. Synlett, 2018, 29, 51-56.	1.0	7
83	Colorimetric Calcium Probe with Comparison to an Ion-Selective Optode. ACS Omega, 2018, 3, 12476-12481.	1.6	6
84	A Computational Study of Asymmetric Hydrogenation of <scp>2â€Phenyl</scp> Acrylic Acids Catalyzed by a Rh(I) Catalyst with Ferrocenyl Chiral Bisphosphorus Ligand: The Role of <scp>Ionâ€Pair</scp> Interaction^{â€}. Chinese Journal of Chemistry, 2021, 39, 1616-1624.	2.6	4
85	AgN₃-Catalyzed Hydroazidation of Terminal Alkynes and Mechanistic Studies. Chinese Journal of Organic Chemistry, 2020, 40, 2603.	0.6	0