## Lung-Wa Chung

List of Publications by Year in descending order

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76326 82547 5,426 85 40 72 citations h-index g-index papers 96 96 96 6038 docs citations times ranked citing authors all docs

#	Article	IF	CITATIONS
1	Ir-Catalyzed Asymmetric Hydrogenation of Unprotected Indoles: Scope Investigations and Mechanistic Studies. CCS Chemistry, 2023, 5, 1398-1410.	7.8	10
2	New Tricks for an Old Dog: Grubbs Catalysts Enable Efficient Hydrogen Production from Aqueous-Phase Methanol Reforming. ACS Catalysis, 2022, 12, 2212-2222.	11.2	21
3	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.	15.6	18
4	Rhodium(I) Carbeneâ€Promoted Enantioselective Câ^'H Functionalization of Simple Unprotected Indoles, Pyrroles and Heteroanalogues: New Mechanistic Insights. Angewandte Chemie - International Edition, 2022, 61, .	13.8	11
5	Asymmetric Total Synthesis of Phomarol. CCS Chemistry, 2021, 3, 348-357.	7.8	9
6	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.	13.7	61
7	$\hat{l}^2$ -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. Journal of the American Chemical Society, 2021, 143, 3519-3535.	13.7	34
8	Enantioselective Hydrogenation of Tetrasubstituted α,βâ€Unsaturated Carboxylic Acids Enabled by Cobalt(II) Catalysis: Scope and Mechanistic Insights. Angewandte Chemie, 2021, 133, 11485-11491.	2.0	15
9	Enantioselective Hydrogenation of Tetrasubstituted α,βâ€Unsaturated Carboxylic Acids Enabled by Cobalt(II) Catalysis: Scope and Mechanistic Insights. Angewandte Chemie - International Edition, 2021, 60, 11384-11390.	13.8	58
10	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 <sup>â€</sup> . Chinese Journal of Chemistry, 2021, 39, 1616-1624.	4.9	4
11	Multiscale Quantum Refinement Approaches for Metalloproteins. Journal of Chemical Theory and Computation, 2021, 17, 3783-3796.	5.3	8
12	Water as a Direct Proton Source for Asymmetric Hydroarylation Catalyzed by a Rh(I)–Diene: Access to Nonproteinogenic β2/γ2/ΰ2-Amino Acid Derivatives. Organic Letters, 2021, 23, 571-577.	4.6	9
13	Ru-Catalyzed Geminal Hydroboration of Silyl Alkynes via a New <i>gem</i> -Addition Mechanism. Journal of the American Chemical Society, 2020, 142, 13867-13877.	13.7	46
14	N-Bridged Pincer Iridium Complexes for Highly Efficient Alkane Dehydrogenation and the Relevant Linker Effects. ACS Catalysis, 2020, 10, 6475-6487.	11.2	25
15	Unusual KIE and dynamics effects in the Fe-catalyzed hetero-Diels-Alder reaction of unactivated aldehydes and dienes. Nature Communications, 2020, 11, 1850.	12.8	30
16	Asymmetric synthesis of quaternary $\hat{l}$ ±-trifluoromethyl $\hat{l}$ ±-amino acids by Ir-catalyzed allylation followed by kinetic resolution. Chemical Communications, 2020, 56, 3333-3336.	4.1	22
17	AgN <sub>3</sub> -Catalyzed Hydroazidation of Terminal Alkynes and Mechanistic Studies. Chinese Journal of Organic Chemistry, 2020, 40, 2603.	1.3	0
18	Ru-Catalyzed Migratory Geminal Semihydrogenation of Internal Alkynes to Terminal Olefins. Journal of the American Chemical Society, 2019, 141, 17441-17451.	13.7	38

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19	Novel Molecular Doping Mechanism for nâ€Doping of SnO <sub>2</sub> via Triphenylphosphine Oxide and Its Effect on Perovskite Solar Cells. Advanced Materials, 2019, 31, e1805944.	21.0	152
20	Asymmetric Total Synthesis of Cerorubenic Acid-III. Journal of the American Chemical Society, 2019, 141, 2872-2877.	13.7	30
21	Exploiting the trifluoroethyl group as a precatalyst ligand in nickel-catalyzed Suzuki-type alkylations. Chemical Science, 2019, 10, 5275-5282.	7.4	14
22	Enantioselective Rhodium-Catalyzed Cycloisomerization of 1,6-Allenynes to access 5/6-Fused Bicycle [4.3.0] nonadienes. Nature Communications, 2019, 10, 949.	12.8	16
23	A Missing Piece of the Mechanism in Metal-Catalyzed Hydrogenation: Co(â^'l)/Co(0)/Co(+l) Catalytic Cycle for Co(â^'l)-Catalyzed Hydrogenation. Organic Letters, 2019, 21, 360-364.	4.6	19
24	Kinetic Resolution of Alkylidene Norcamphors via a Ligand-Controlled Umpolung-Type 1,3-Dipolar Cycloaddition. IScience, 2019, 11, 146-159.	4.1	25
25	Mechanistic insights into asymmetric reductive coupling of isoquinolines by a chiral diboron with DFT calculations. Journal of Organometallic Chemistry, 2018, 864, 97-104.	1.8	13
26	Catalytic asymmetric trifluoromethylthiolation of carbonyl compounds <i>via </i> a diastereo and enantioselective Cu-catalyzed tandem reaction. Chemical Communications, 2018, 54, 4581-4584.	4.1	33
27	Computational Insights into the Reaction Mechanisms of Nickelâ€Catalyzed Hydrofunctionalizations and Nickelâ€Dependent Enzymes. Asian Journal of Organic Chemistry, 2018, 7, 522-536.	2.7	12
28	Rhodium-catalyzed asymmetric hydrogenation of $\hat{l}^2$ -cyanocinnamic esters with the assistance of a single hydrogen bond in a precise position. Chemical Science, 2018, 9, 1919-1924.	7.4	35
29	Br $ ilde{A}_i$ 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.	4.6	62
30	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.	13.7	64
31	Enantioselective Palladium-Catalyzed Decarboxylative Allylation of $\hat{I}^2$ -Keto Esters Assisted by a Thiourea. Synlett, 2018, 29, 51-56.	1.8	7
32	Development of a novel secondary phosphine oxide–ruthenium( <scp>ii</scp> ) catalyst and its application for carbonyl reduction. Chemical Communications, 2018, 54, 535-538.	4.1	18
33	Colorimetric Calcium Probe with Comparison to an Ion-Selective Optode. ACS Omega, 2018, 3, 12476-12481.	3.5	6
34	Silicon-oriented regio- and enantioselective rhodium-catalyzed hydroformylation. Nature Communications, 2018, 9, 2045.	12.8	28
35	A Combined DFT/IM-MS Study on the Reaction Mechanism of Cationic Ru(II)-Catalyzed Hydroboration of Alkynes. ACS Catalysis, 2017, 7, 1361-1368.	11.2	56
36	Iridium-Catalyzed Asymmetric Hydrogenation of Ketones with Accessible and Modular Ferrocene-Based Amino-phosphine Acid (f-Ampha) Ligands. Organic Letters, 2017, 19, 690-693.	4.6	79

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37	Enantioselective palladium-catalyzed diboration of 1,1-disubstituted allenes. Chemical Science, 2017, 8, 5161-5165.	7.4	51
38	Enzymeâ€Inspired Chiral Secondaryâ€Phosphineâ€Oxide Ligand with Dual Noncovalent Interactions for Asymmetric Hydrogenation. Angewandte Chemie, 2017, 129, 6912-6916.	2.0	22
39	Enzymeâ€Inspired Chiral Secondaryâ€Phosphineâ€Oxide Ligand with Dual Noncovalent Interactions for Asymmetric Hydrogenation. Angewandte Chemie - International Edition, 2017, 56, 6808-6812.	13.8	60
40	Organocatalytic atroposelective synthesis of axially chiral styrenes. Nature Communications, 2017, 8, 15238.	12.8	128
41	Reaction Mechanism of Cu(I)-Mediated Reductive CO <sub>2</sub> Coupling for the Selective Formation of Oxalate: Cooperative CO <sub>2</sub> Reduction To Give Mixed-Valence Cu <sub>2</sub> (CO <sub>2</sub> <sup>•–</sup> ) and Nucleophilic-Like Attack. Inorganic Chemistry, 2017. 56. 6809-6819.	4.0	39
42	Guestâ€Induced Folding and Selfâ€Assembly of Conformationally Adaptive Macrocycles into Nanosheets and Nanotubes. Chemistry - A European Journal, 2017, 23, 1516-1520.	3.3	19
43	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.	13.7	26
44	Practical and Asymmetric Reductive Coupling of Isoquinolines Templated by Chiral Diborons. Journal of the American Chemical Society, 2017, 139, 9767-9770.	13.7	54
45	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.	7.4	71
46	Nickel-catalyzed asymmetric hydrogenation of $\hat{l}^2$ -acylamino nitroolefins: an efficient approach to chiral amines. Chemical Science, 2017, 8, 6419-6422.	7.4	82
47	Alternative Mechanistic Strategy for Enzyme Catalysis in a Niâ€Dependent Lactate Racemase (LarA): Intermediate Destabilization by the Cofactor. Chemistry - A European Journal, 2017, 23, 3623-3630.	3.3	28
48	Multiscale Simulations on Spectral Tuning and the Photoisomerization Mechanism in Fluorescent RNA Spinach. Journal of Chemical Theory and Computation, 2016, 12, 5453-5464.	5.3	11
49	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.	11.2	75
50	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.	15.6	100
51	Hydrogenation of Aldehydes Catalyzed by an Available Ruthenium Complex. Organic Letters, 2016, 18, 1518-1521.	4.6	39
52	Mechanism of Ni-NHC Catalyzed Hydrogenolysis of Aryl Ethers: Roles of the Excess Base. ACS Catalysis, 2016, 6, 483-493.	11,2	76
53	Ferrocenyl chiral bisphosphorus ligands for highly enantioselective asymmetric hydrogenation via noncovalent ion pair interaction. Chemical Science, 2016, 7, 6669-6673.	7.4	60
54	Computational Organic Chemistry: Bridging Theory and Experiment in Establishing the Mechanisms of Chemical Reactions. Journal of the American Chemical Society, 2015, 137, 1706-1725.	13.7	271

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55	Highly Regio―and Stereoselective Hydrosilylation of Internal Thioalkynes under Mild Conditions. Angewandte Chemie - International Edition, 2015, 54, 5632-5635.	13.8	77
56	The ONIOM Method and Its Applications. Chemical Reviews, 2015, 115, 5678-5796.	47.7	936
57	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.	5.3	16
58	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.	5.3	17
59	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.	3.2	44
60	Dearomative Indole [5+2] Cycloaddition Reactions: Stereoselective Synthesis of Highly Functionalized Cyclohepta[ <i>b</i> ) indoles. Angewandte Chemie - International Edition, 2014, 53, 11051-11055.	13.8	77
61	Ligand-Controlled Remarkable Regio- and Stereodivergence in Intermolecular Hydrosilylation of Internal Alkynes: Experimental and Theoretical Studies. Journal of the American Chemical Society, 2013, 13835-13842.	13.7	135
62	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.	2.6	29
63	The ONIOM method: its foundation and applications to metalloenzymes and photobiology. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 327-350.	14.6	173
64	Mechanistic Studies on the Reversible Hydrogenation of Carbon Dioxide Catalyzed by an Ir-PNP Complex. Organometallics, 2011, 30, 6742-6750.	2.3	288
65	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.	13.7	63
66	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.	13.7	52
67	Photodynamics of All- <i>trans</i> Retinal Protonated Schiff Base in Bacteriorhodopsin and Methanol Solution. Journal of Chemical Theory and Computation, 2011, 7, 2694-2698.	5.3	30
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.	3.3	16
69	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.	2.6	37
70	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.	2.6	69
71	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.	13.7	78
72	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.	13.7	74

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73	Primary Events of Photodynamics in Reversible Photoswitching Fluorescent Protein Dronpa. Journal of Physical Chemistry Letters, 2010, 1, 3328-3333.	4.6	51
74	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.	13.7	146
75	DFT and ONIOM(DFT:MM) Studies on Coâ^'C Bond Cleavage and Hydrogen Transfer in B <sub>12</sub> -Dependent Methylmalonyl-CoA Mutase. Stepwise or Concerted Mechanism?. Journal of the American Chemical Society, 2009, 131, 5115-5125.	13.7	53
76	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.	13.7	88
77	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.	13.7	80
78	A Theoretical Study on the <i>trans</i> -Addition Intramolecular Hydroacylation of 4-Alkynals Catalyzed by Cationic Rhodium Complexes. Journal of Organic Chemistry, 2008, 73, 2649-2655.	<b>3.2</b>	27
79	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.	3.2	33
80	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.	3.2	81
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	Theoretical Study of the Intrinsic Reactivities of Various Allylmetals toward Carbonyls and Water. Organometallics, 2005, 24, 1598-1607.	2.3	21
83	Experimental and Theoretical Studies of the Propargyl-Allenylindium System. Journal of the American Chemical Society, 2004, 126, 13326-13334.	13.7	53
84	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.	13.7	156
85	Highly efficient and practical resolution of $1,1\hat{a}\in^2$ -spirobiindane-7,7 $\hat{a}\in^2$ -diol by inclusion crystallization with N-benzylcinchonidinium chloride. Tetrahedron: Asymmetry, 2002, 13, 1363-1366.	1.8	91