Shi-Lu Chen

List of Publications by Year
in descending order

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62	1,807	257450	276875
papers	citations	24 h-index	41 g-index

62	62	62	2078
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Significant van der Waals Effects in Transition Metal Complexes. Journal of Chemical Theory and Computation, 2010, 6, 2040-2044.	5.3	185
2	Theoretical Study of the Phosphotriesterase Reaction Mechanism. Journal of Physical Chemistry B, 2007, 111, 1253-1255.	2.6	105
3	An Ironâ€Containing Metalâ€“Organic Framework as a Highly Efficient Catalyst for Ozone Decomposition. Angewandte Chemie - International Edition, 2018, 57, 16416-16420.	13.8	97
4	A General and Extremely Simple Remote Approach toward Graphene Bulks with In Situ Multifunctionalization. Advanced Materials, 2016, 28, 3305-3312.	21.0	79
5	Nitrogen-doped porous carbon monolith as a highly efficient catalyst for CO₂conversion. Journal of Materials Chemistry A, 2014, 2, 18360-18366.	10.3	75
6	An Ironâ€Containing Metalâ€“Organic Framework as a Highly Efficient Catalyst for Ozone Decomposition. Angewandte Chemie, 2018, 130, 16654-16658.	2.0	73
7	Peptide Hydrolysis by the Binuclear Zinc Enzyme Aminopeptidase from Aeromonas proteolytica:â€‰ A Density Functional Theory Study. Journal of Physical Chemistry B, 2008, 112, 2494-2500.	2.6	68
8	Technical aspects of quantum chemical modeling of enzymatic reactions: the case of phosphotriesterase. Theoretical Chemistry Accounts, 2008, 120, 515-522.	1.4	67
9	Structure of Diethyl Phosphate Bound to the Binuclear Metal Center of Phosphotriesterase. Biochemistry, 2008, 47, 9497-9504.	2.5	67
10	Aerobic oxidative cyclization of benzamides via meta-selective Câ€“H tert-alkylation: rapid entry to 7-alkylated isoquinolinediones. Chemical Communications, 2016, 52, 4470-4473.	4.1	62
11	Unactivated C(sp³)â€“H Bond Functionalization of Alkyl Nitriles with Vinylarenes and Mechanistic Studies. Organic Letters, 2016, 18, 5986-5989.	4.6	53
12	Efficient biosynthesis of heterodimeric C3-aryl pyrroloindoline alkaloids. Nature Communications, 2018, 9, 4428.	12.8	53
13	Cucurbit[7]uril-Carbazole Two-Photon Photoinitiators for the Fabrication of Biocompatible Three-Dimensional Hydrogel Scaffolds by Laser Direct Writing in Aqueous Solutions. ACS Applied Materials & Interfaces, 2019, 11, 1782-1789.	8.0	52
14	How Is Methane Formed and Oxidized Reversibly When Catalyzed by Niâ€Containing Methylâ€Coenzyme M Reductase?. Chemistry - A European Journal, 2012, 18, 6309-6315.	3.3	45
15	How Is a Co-Methyl Intermediate Formed in the Reaction of Cobalamin-Dependent Methionine Synthase? Theoretical Evidence for a Two-Step Methyl Cation Transfer Mechanism. Journal of Physical Chemistry B, 2011, 115, 4066-4077.	2.6	44
16	Copper-catalyzed radical cascades of para-quinone methides with AIBN and H2O via Î±-cyanoalkylation by Câ€“C bond cleavage: new access to benzofuran-2(3H)-ones. Chemical Communications, 2019, 55, 4578-4581.	4.1	44
17	Reaction mechanism of the binuclear zinc enzyme glyoxalase II â€“ A theoretical study. Journal of Inorganic Biochemistry, 2009, 103, 274-281.	3.5	41
18	Is There a Ni-Methyl Intermediate in the Mechanism of Methyl-Coenzyme M Reductase?. Journal of the American Chemical Society, 2009, 131, 9912-9913.	13.7	37

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19	Functional Porous Organic Polymers Comprising a Triaminotriphenylazobenzene Subunit as a Platform for Copper-Catalyzed Aerobic Câ€“H Oxidation. Chemistry of Materials, 2019, 31, 5421-5430.	6.7	37
20	Azo-linked porous organic polymers: robust and time-efficient synthesisviaNaBH₄-mediated reductive homocoupling on polynitro monomers and adsorption capacity towards aniline in water. Journal of Materials Chemistry A, 2018, 6, 5608-5612.	10.3	36
21	Which Oxidation State Initiates Dehalogenation in the B12-Dependent Enzyme NpRdhA: Co^{II}, Co^I, or Co⁰?. ACS Catalysis, 2015, 5, 7350-7358.	11.2	35
22	An investigation of possible competing mechanisms for Ni-containing methylâ€“coenzyme M reductase. Physical Chemistry Chemical Physics, 2014, 16, 14029.	2.8	28
23	Phosphate Monoester Hydrolysis by Trinuclear Alkaline Phosphatase; DFT Study of Transition States and Reaction Mechanism. ChemPhysChem, 2014, 15, 2321-2330.	2.1	27
24	Unraveling the Mechanism and Regioselectivity of the B12â€Dependent Reductive Dehalogenase PceA. Chemistry - A European Journal, 2016, 22, 12391-12399.	3.3	25
25	The Decarboxylation of Î±,Î²-Unsaturated Acid Catalyzed by Prenylated FMN-Dependent Ferulic Acid Decarboxylase and the Enzyme Inhibition. Journal of Organic Chemistry, 2016, 81, 9289-9295.	3.2	25
26	Include Dispersion in Quantum Chemical Modeling of Enzymatic Reactions: The Case of Isoaspartyl Dipeptidase. Journal of Chemical Theory and Computation, 2015, 11, 2525-2535.	5.3	23
27	Radical 1,4â€Aryl Migration Enabled Remote Crossâ€Electrophile Coupling of Î±â€Aminoâ€Î²â€Bromo Acid Esters with Aryl Bromides. Angewandte Chemie - International Edition, 2021, 60, 21360-21367.	13.8	22
28	A dominant homolytic Oâ€“Cl bond cleavage with low-spin triplet-state Fe(<scp>iv</scp>)îŠO formed is revealed in the mechanism of heme-dependent chlorite dismutase. Dalton Transactions, 2014, 43, 973-981.	3.3	21
29	From NAD⁺ to Nickel Pincer Complex: A Significant Cofactor Evolution Presented by Lactate Racemase. Chemistry - A European Journal, 2017, 23, 7545-7557.	3.3	20
30	Porous platinumâ€“silver bimetallic alloys: surface composition and strain tunability toward enhanced electrocatalysis. Nanoscale, 2018, 10, 21703-21711.	5.6	20
31	Using Machine Learning to Predict the Dissociation Energy of Organic Carbonyls. Journal of Physical Chemistry A, 2020, 124, 3844-3850.	2.5	18
32	Theoretical investigation of astacin proteolysis. Journal of Inorganic Biochemistry, 2012, 111, 70-79.	3.5	17
33	How does the silicon element perform in JD-dyes: a theoretical investigation. Journal of Materials Chemistry A, 2015, 3, 8308-8315.	10.3	16
34	Theoretical Studies of Nickel-Dependent Enzymes. Inorganics, 2019, 7, 95.	2.7	15
35	High-valent cationic metalâ€“organic macrocycles as novel supports for immobilization and enhancement of activity of polyoxometalate catalysts. Catalysis Science and Technology, 2016, 6, 8540-8547.	4.1	14
36	Asymmetric abstraction of two chemically-equivalent methylene hydrogens: significant enantioselectivity of endoperoxide presented by fumitremorgin B endoperoxidase. Physical Chemistry Chemical Physics, 2018, 20, 26500-26505.	2.8	13

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37	A Copper (II) Acetate Mediated Oxidativeâ€Coupling of Styrenes and Ethers Through an Unactivated C(sp³)â^'H Bond Functionalization. Advanced Synthesis and Catalysis, 2019, 361, 1007-1011.	4.3	13
38	How To Produce Methane Precursor in the Upper Ocean by An Untypical Nonâ€Heme Feâ€Dependent Methylphosphonate Synthase?. ChemPhysChem, 2020, 21, 385-396.	2.1	12
39	Significant electron transfer in heme catalysis: The case of chlorite dismutase. Journal of Catalysis, 2017, 348, 40-46.	6.2	11
40	How does Mo-dependent perchlorate reductase work in the decomposition of oxyanions?. Dalton Transactions, 2019, 48, 5683-5691.	3.3	11
41	Insights into the Chemical Reactivity in Acetyl-CoA Synthase. Inorganic Chemistry, 2020, 59, 15167-15179.	4.0	11
42	Irreversible tautomerization as a powerful tool to access unprecedented functional porous organic polymers with a tris(Î²-keto-hydrazo)cyclohexane subunit (TKH-POPs). Chemical Communications, 2020, 56, 2103-2106.	4.1	10
43	A Key Piece in the Global N-Cycle: The Nâ€“N Bond Formation Presented by Heme-Dependent Hydrazine Synthase. ACS Catalysis, 2021, 11, 6489-6498.	11.2	9
44	From Alkane to Alkene: The Inert Aliphatic Câ€“H Bond Activation Presented by Binuclear Iron Stearoyl-CoA Desaturase with a Long di-Fe Distance of 6 Ã…. ACS Catalysis, 2019, 9, 4345-4359.	11.2	8
45	An Unprecedented Ring-Contraction Mechanism in Cobalamin-Dependent Radical S-Adenosylmethionine Enzymes. Journal of Physical Chemistry Letters, 2020, 11, 6812-6818.	4.6	8
46	Enzymatic N N bond formation: Mechanism for the N-nitroso synthesis catalyzed by non-heme iron SznF enzyme. Journal of Catalysis, 2021, 398, 44-53.	6.2	7
47	Î¼₃-Oxo stabilized by three metal cations is a sufficient nucleophile for enzymatic hydrolysis of phosphate monoesters. Dalton Transactions, 2016, 45, 2517-2522.	3.3	6
48	Theoretical study on reaction mechanism of sulfuric acid and ammonia and hydration of (NH4)2SO4. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	5
49	How is DMSP decomposed when catalyzed by RlDddP binuclear iron DMSP lyase?. Journal of Catalysis, 2018, 360, 1-8.	6.2	5
50	Unusual Assembly and Conversion of Graphene Quantum Dots into Crystalline Graphite Nanocapsules. Chemistry - an Asian Journal, 2017, 12, 1272-1276.	3.3	4
51	Mechanism and Inhibitor Exploration with Binuclear Mg Ketolâ€Acid Reductoisomerase: Targeting the Biosynthetic Pathway of Branchedâ€Chain Amino Acids. ChemBioChem, 2020, 21, 381-391.	2.6	4
52	Facile synthesis of a porous polynorbornene with an azobenzene subunit: selective adsorption of 4-nitrophenol over 4-aminophenol in water. Polymer Chemistry, 2020, 11, 6429-6434.	3.9	4
53	Syndiospecific Polymerization of o-Methoxystyrene and Its Silyloxy or Fluorine-Substituted Derivatives by HNC-Ligated Scandium Catalysts: Synthesis of Ultrahigh-Molecular-Weight Functionalized Polymers. Macromolecules, 2021, 54, 10838-10849.	4.8	4
54	Exothermic or Endothermic Decomposition of Disubstituted Tetrazoles Tuned by Substitution Fashion and Substituents. Journal of Physical Chemistry A, 2018, 122, 8-15.	2.5	3

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55	Key Piece in the Wolfe Cycle of Methanogenesis: The Sâ€“S Bond Dissociation Conducted by Noncubane [Fe₄S₄] Cluster-Dependent Heterodisulfide Reductase. ACS Catalysis, 2022, 12, 2606-2622.	11.2	3
56	How does binuclear zinc amidohydrolase FwdA work in the initial step of methanogenesis: From formate to formyl-methanofuran. Journal of Inorganic Biochemistry, 2018, 185, 71-79.	3.5	2
57	Theoretical Study of VX Hydrolysis Mechanism Catalyzed by Phosphotriesterase Mutant H254R. ChemistrySelect, 2020, 5, 8986-8991.	1.5	2
58	Highly magnetically responsive porous nanoparticles based on tris(Î²-keto-hydrazo)-cyclohexane subunit: Fast removal of dyes from water with convenient recyclability. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 648, 129173.	4.7	2
59	Theoretical study of aromatic hydroxylation of the [Cu2(H-XYL)O2]2+ complex mediated by a side-on peroxo dicopper core and Cu-ligand effects. Dalton Transactions, 2019, 48, 16882-16893.	3.3	1
60	Handling methane: a Ni(<scp>i</scp>) F₄₃₀-like cofactor derived from VB₁₂ is active in methyl-coenzyme M reductase. Chemical Communications, 2021, 57, 476-479.	4.1	1
61	Radical 1,4â€Aryl Migration Enabled Remote Crossâ€Electrophile Coupling of Î±â€Aminoâ€Î²â€Bromo Acid Esters with Aryl Bromides. Angewandte Chemie, 2021, 133, 21530-21537.	2.0	1
62	Functionalization Methodology for Synthesis of Silane-End-Functionalized Linear and Star Poly(aryl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 Macromolecules, 0, , .	4.8	1