Xi-Chen Li

List of Publications by Year
in descending order

34 papers	569 citations	840776 11 h-index	642732 23 g-index
35 all docs	35 docs citations	35 times ranked	917 citing authors

#	Article	IF	Citations
1	Reorienting Mechanism of Harderoheme in Coproheme Decarboxylaseâ€"A Computational Study. International Journal of Molecular Sciences, 2022, 23, 2564.	4.1	4
2	Interactive Regulation between Aliphatic Hydroxylation and Aromatic Hydroxylation of Thaxtomin D in TxtC: A Theoretical Investigation. Inorganic Chemistry, 2021, 60, 6433-6445.	4.0	5
3	N-Nitrosation Mechanism Catalyzed by Non-heme Iron-Containing Enzyme SznF Involving Intramolecular Oxidative Rearrangement. Inorganic Chemistry, 2021, 60, 7719-7731.	4.0	4
4	Theoretical Studies on the Binding Mode and Reaction Mechanism of TLP Hydrolase ŀpHIUH. Molecules, 2021, 26, 3884.	3.8	0
5	Theoretical study on the catalytic mechanism of human deoxyhypusine hydroxylase. Physical Chemistry Chemical Physics, 2020, 22, 22736-22745.	2.8	6
6	A Theoretical Study of the Recently Suggested Mn^{VII} Mechanism for Oâ€"O Bond Formation in Photosystem II. Journal of Physical Chemistry A, 2020, 124, 8011-8018.	2.5	8
7	Ruffling drives coproheme decarboxylation by facilitating PCET: a theoretical investigation of ChdC. Physical Chemistry Chemical Physics, 2020, 22, 16117-16124.	2.8	7
8	ONIOM investigations of the heme degradation mechanism by MhuD: the critical function of heme ruffling. Physical Chemistry Chemical Physics, 2020, 22, 8817-8826.	2.8	7
9	Theoretical Study of the Mechanisms of Two Copper Water Oxidation Electrocatalysts with Bipyridine Ligands. ACS Catalysis, 2019, 9, 8798-8809.	11.2	9
10	Theoretical study of the mechanism of the manganese catalase KatB. Journal of Biological Inorganic Chemistry, 2019, 24, 103-115.	2.6	4
11	A theoretical study on oxidative cleavage of olefins to carbonyls catalysed by Fe(<scp>iii</scp>)-PyBisulidine. Dalton Transactions, 2017, 46, 3825-3832.	3.3	3
12	Function Coupling Mechanism of PhuS and HemO in Heme Degradation. Scientific Reports, 2017, 7, 11273.	3.3	6
13	Cluster size convergence for the energetics of the oxygen evolving complex in PSII. Journal of Computational Chemistry, 2017, 38, 2157-2160.	3.3	6
14	Distal Proton Shuttle Mechanism of Ribosome Catalysed Peptide Bond Formationâ€"A Theoretical Study. Molecules, 2017, 22, 571.	3.8	5
15	Theoretical studies of the function switch and mechanism of AceK as a highly active ATPase. RSC Advances, 2016, 6, 68120-68127.	3.6	1
16	Ruthenium(II) Complexes of Aryl Triazole Foldamers as Receptors for Anions. Chemistry - A European Journal, 2016, 22, 5233-5242.	3.3	17
17	Aryl-triazole foldamers incorporating a pyridinium motif for halide anion binding in aqueous media. Chemical Communications, 2016, 52, 4505-4508.	4.1	26
18	Water Oxidation for Simplified Models of the Oxygenâ€Evolving Complex in Photosystemâ€...II. Chemistry - A European Journal, 2015, 21, 18821-18827.	3.3	11

#	Article	IF	Citations
19	Molecular Dynamics Simulation Studies of dTTP Binding and Catalysis Mediated by YhdE Dimerization. PLoS ONE, 2015, 10, e0134879.	2.5	7
20	Simulation of the isotropic EXAFS spectra for the S ₂ and S ₃ structures of the oxygen evolving complex in photosystem II. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 3979-3984.	7.1	32
21	Alternative mechanisms for O₂release and Oâ€“O bond formation in the oxygen evolving complex of photosystem II. Physical Chemistry Chemical Physics, 2015, 17, 12168-12174.	2.8	97
22	Phosphoryl transfer reaction catalyzed by membrane diacylglycerol kinase: a theoretical mechanism study. Physical Chemistry Chemical Physics, 2015, 17, 25228-25234.	2.8	1
23	Reaction Mechanism of Water Oxidation Catalyzed by Iron Tetraamido Macrocyclic Ligand Complexes â€“ A DFT Study. European Journal of Inorganic Chemistry, 2014, 2014, 728-741.	2.0	61
24	Theoretical EXAFS studies of a model of the oxygenâ€evolving complex of photosystem II obtained with the quantum cluster approach. International Journal of Quantum Chemistry, 2013, 113, 474-478.	2.0	26
25	Water Oxidation Mechanism for Synthetic Coâ€“Oxides with Small Nuclearity. Journal of the American Chemical Society, 2013, 135, 13804-13813.	13.7	106
26	Unique Kinase Catalytic Mechanism of AceK with a Single Magnesium Ion. PLoS ONE, 2013, 8, e72048.	2.5	7
27	A comparison between artificial and natural water oxidation. Dalton Transactions, 2011, 40, 11296.	3.3	34
28	DFT studies of the degradation mechanism of methyl mercury activated by a sulfur-rich ligand. Physical Chemistry Chemical Physics, 2010, 12, 3961.	2.8	13
29	Catalytic activities of dismution reactions of Cu(bpy)Br2 compound and its derivatives as SOD mimics: A theoretical study. Journal of Molecular Modeling, 2009, 15, 1397-1405.	1.8	4
30	Energy basis of recognition of base pair for platinum-based antitumour drug ZD0473 and cisplatin. Science in China Series B: Chemistry, 2008, 51, 359-366.	0.8	2
31	Evaluation of Amber force field parameters for copper(II) with pyridylmethyl-amine and benzimidazolylmethyl-amine ligands: A quantum chemical study. Chemical Physics Letters, 2008, 455, 354-360.	2.6	27
32	Theoretical exploration of the cooperative effect in NMFâ€“NMFâ€“amino acid residue hydrogen bonding system. Physical Chemistry Chemical Physics, 2008, 10, 5607.	2.8	6
33	Theoretical study on stabilities of multiple hydrogen bonded dimers. Physical Chemistry Chemical Physics, 2006, 8, 4427.	2.8	16
34	Theoretical investigation on the reaction mechanism of UTP cyclohydrolase. Physical Chemistry Chemical Physics, 0, , .	2.8	1