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	Water Oxidation Mechanism for Synthetic Coâ€“Oxides with Small Nuclearity. Journal of the American Chemical Society, 2013, 135, 13804-13813.	13.7	106
2	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
3	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
4	A comparison between artificial and natural water oxidation. Dalton Transactions, 2011, 40, 11296.	3.3	34
5	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
6	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
7	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
8	Aryl-triazole foldamers incorporating a pyridinium motif for halide anion binding in aqueous media. Chemical Communications, 2016, 52, 4505-4508.	4.1	26
9	Ruthenium(II) Complexes of Aryl Triazole Foldamers as Receptors for Anions. Chemistry - A European Journal, 2016, 22, 5233-5242.	3.3	17
10	Theoretical study on stabilities of multiple hydrogen bonded dimers. Physical Chemistry Chemical Physics, 2006, 8, 4427.	2.8	16
11	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
12	Water Oxidation for Simplified Models of the Oxygenâ€Evolving Complex in Photosystemâ€…II. Chemistry - A European Journal, 2015, 21, 18821-18827.	3.3	11
13	Theoretical Study of the Mechanisms of Two Copper Water Oxidation Electrocatalysts with Bipyridine Ligands. ACS Catalysis, 2019, 9, 8798-8809.	11.2	9
14	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
15	Molecular Dynamics Simulation Studies of dTTP Binding and Catalysis Mediated by YhdE Dimerization. PLoS ONE, 2015, 10, e0134879.	2.5	7
16	Ruffling drives coproheme decarboxylation by facilitating PCET: a theoretical investigation of ChdC. Physical Chemistry Chemical Physics, 2020, 22, 16117-16124.	2.8	7
17	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
18	Unique Kinase Catalytic Mechanism of AceK with a Single Magnesium Ion. PLoS ONE, 2013, 8, e72048.	2.5	7

#	Article	IF	Citations
19	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
20	Function Coupling Mechanism of PhuS and HemO in Heme Degradation. Scientific Reports, 2017, 7, 11273.	3.3	6
21	Cluster size convergence for the energetics of the oxygen evolving complex in PSII. Journal of Computational Chemistry, 2017, 38, 2157-2160.	3.3	6
22	Theoretical study on the catalytic mechanism of human deoxyhypusine hydroxylase. Physical Chemistry Chemical Physics, 2020, 22, 22736-22745.	2.8	6
23	Distal Proton Shuttle Mechanism of Ribosome Catalysed Peptide Bond Formationâ€”A Theoretical Study. Molecules, 2017, 22, 571.	3.8	5
24	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
25	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
26	Theoretical study of the mechanism of the manganese catalase KatB. Journal of Biological Inorganic Chemistry, 2019, 24, 103-115.	2.6	4
27	N-Nitrosation Mechanism Catalyzed by Non-heme Iron-Containing Enzyme SznF Involving Intramolecular Oxidative Rearrangement. Inorganic Chemistry, 2021, 60, 7719-7731.	4.0	4
28	Reorienting Mechanism of Harderoheme in Coproheme Decarboxylaseâ€”A Computational Study. International Journal of Molecular Sciences, 2022, 23, 2564.	4.1	4
29	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
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	Phosphoryl transfer reaction catalyzed by membrane diacylglycerol kinase: a theoretical mechanism study. Physical Chemistry Chemical Physics, 2015, 17, 25228-25234.	2.8	1
32	Theoretical studies of the function switch and mechanism of AceK as a highly active ATPase. RSC Advances, 2016, 6, 68120-68127.	3.6	1
33	Theoretical investigation on the reaction mechanism of UTP cyclohydrolase. Physical Chemistry Chemical Physics, 0, , .	2.8	1
34	Theoretical Studies on the Binding Mode and Reaction Mechanism of TLP Hydrolase kpHIUH. Molecules, 2021, 26, 3884.	3.8	0