Assocâ€Prof Lin Cheng

List of Publications by Year
in descending order

39 papers	568 citations	759233 12 h-index	677142 22 g-index
39 all docs	39 docs citations	39 times ranked	717 citing authors

#	Article	IF	Citations
1	Enhanced visible-light photocatalytic activity of carbonate-doped anatase TiO2 based on the electron-withdrawing bidentate carboxylate linkage. Applied Catalysis B: Environmental, 2017, 202, 642-652.	20.2	125
2	Mechanistic Insight into the Alcohol Oxidation Mediated by an Efficient Green [CuBr₂(2,2â€²-bipy)]-TEMPO Catalyst by Density Functional Method. Inorganic Chemistry, 2010, 49, 9392-9399.	4.0	47
3	Structural Stability and Evolution of Scandium-Doped Silicon Clusters: Evolution of Linked to Encapsulated Structures and Its Influence on the Prediction of Electron Affinities for ScSi_n (n = 4â€“16) Clusters. Inorganic Chemistry, 2018, 57, 12934-12940.	4.0	39
4	Electronic structures and chemical bonding in 4d transition metal monohalides. Journal of Computational Chemistry, 2007, 28, 2190-2202.	3.3	33
5	RuN₄ Doped Graphene Oxide, a Highly Efficient Bifunctional Catalyst for Oxygen Reduction and CO₂ Reduction from Computational Study. ACS Sustainable Chemistry and Engineering, 2019, 7, 8136-8144.	6.7	29
6	Mechanistic insight into alcohol oxidation mediated by an efficient green CuII-bipy catalyst with and without TEMPO by density functional methods. Dalton Transactions, 2010, 39, 5377.	3.3	18
7	Regioselective Bis-Selenation of Allenes Catalyzed by Palladium Complexes: A Theoretical Study. Organometallics, 2009, 28, 1506-1513.	2.3	17
8	Theoretical studies on the reaction mechanism of palladium(0)-catalyzed addition of thiocyanates to alkynes. Dalton Transactions, 2008, , 3879.	3.3	15
9	Structural growth pattern of neutral and negatively charged yttrium-doped silicon clusters YSi_n^{0/â^'} (n=6â€“20): from linked to encapsulated structures. RSC Advances, 2019, 9, 2731-2739.	3.6	15
10	Efficient electroreduction of CO2 by single-atom catalysts two-dimensional metal hexahydroxybenzene frameworks: A theoretical study. Applied Surface Science, 2021, 550, 149389.	6.1	15
11	Probing Structure, Thermochemistry, Electron Affinity and Magnetic Moment of Erbium-Doped Silicon Clusters ErSin (nÂ=Â3â€“10) and Their Anions with Density Functional Theory. Journal of Cluster Science, 2018, 29, 301-311.	3.3	14
12	Sulfated Ceâ€doped TiO₂ as visible light driven photocatalyst: Preparation, characterization and promotion effects of Ce doping and sulfation on catalyst performance. Environmental Progress and Sustainable Energy, 2017, 36, 494-504.	2.3	13
13	Theoretical studies on the reaction mechanism of oxidation of primary alcohols by Zn/Cu(ii)-phenoxyl radical catalyst. Dalton Transactions, 2009, , 3286.	3.3	12
14	Fe-porphyrin carbon matrix as a bifunctional catalyst for oxygen reduction and CO₂ reduction from theoretical perspective. Molecular Physics, 2019, 117, 1805-1812.	1.7	12
15	Mechanistic insight into the aerobic oxidation of benzyl alcohol catalyzed by the Cu^{II}â€“TEMPO catalyst in alkaline water solution. RSC Advances, 2015, 5, 83976-83984.	3.6	11
16	The reaction pathways of the oxygen reduction reaction on IrN 4 doped divacancy graphene: A theoretical study. Journal of Molecular Graphics and Modelling, 2018, 80, 293-298.	2.4	11
17	A new natural layered clay mineral applicable to photocatalytic hydrogen production and/or degradation of dye pollutant. Environmental Progress and Sustainable Energy, 2018, 37, 1003-1010.	2.3	11
18	Theoretical study of two-dimensional bis(iminothiolato)metal monolayers as promising electrocatalysts for carbon dioxide reduction. New Journal of Chemistry, 2020, 44, 12299-12306.	2.8	11

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19	Facile synthesis of oxygen-deficient nano-TiO₂coordinated by acetate ligands for enhanced visible-light photocatalytic performance. Catalysis Science and Technology, 2020, 10, 3875-3889.	4.1	11
20	Theoretical Studies on the Reaction Mechanism of Platinum-Catalyzed Diboration of Allenes. Organometallics, 2008, 27, 6464-6471.	2.3	10
21	DFT studies on the mechanism of alcohol oxidation by the (bpy)CuI-TEMPO/NMI catalytic system. Dalton Transactions, 2015, 44, 7395-7403.	3.3	10
22	A Density Functional Theory Study of the Two-Dimensional Bis(iminothiolato)metal Monolayers as Efficient Electrocatalysts for Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2020, 124, 7803-7811.	3.1	10
23	Theoretical studies on the reaction mechanism of alcohol oxidation by high-valent iron-oxo complex of non-heme ligand. Physical Chemistry Chemical Physics, 2010, 12, 4092.	2.8	9
24	A new acidic Ti sol impregnated kaolin photocatalyst: synthesis, characterization and visible light photocatalytic performance. Journal of Sol-Gel Science and Technology, 2013, 65, 204-211.	2.4	9
25	Study on Structural Evolution, Thermochemistry and Electron Affinity of Neutral, Mono- and Di-Anionic Zirconium-Doped Silicon Clusters ZrSin0/-/2- (n = 6â€“16). International Journal of Molecular Sciences, 2019, 20, 2933.	4.1	9
26	Structural stability and evolution of terbiumâ€doped silicon clusters and influence of 4fâ€‰â†’â€‰5d electronic transition mechanism on magnetism and appearance of photoelectron spectroscopy for TbSi_n^{0/â^'} (n = 6â€18) clusters. International Journal of Quantum Chemistry, 2020, 120, e26087.	2.0	9
27	Electrochemical CO₂ Reduction On Two-Dimensional Metal 1,3,5-triamino-2,4,6-Benzenetriol Frameworks: A Density Functional Study. Journal of the Electrochemical Society, 2022, 169, 024513.	2.9	6
28	Reaction mechanism of palladiumâ€catalyzed silastannation of allenes by density functional theory. Journal of Computational Chemistry, 2009, 30, 1521-1531.	3.3	5
29	Revisiting the structural and electronic properties of neutral, monoâ€and diâ€anionic titaniumâ€doped silicon clusters TiSi n 0/â^'/2â^' (n = 6â€16). International Journal of Quantum Chemistry, 2019, 119, e25978.	2.0	5
30	Density functional study on the reaction mechanism of palladiumâ€catalyzed addition of cyanoboranes to alkynes. Journal of Computational Chemistry, 2008, 29, 1825-1839.	3.3	4
31	Mechanism of methylacetylene bisselenation catalyzed by palladium complex from density functional study. Journal of Computational Chemistry, 2011, 32, 1170-1177.	3.3	4
32	DFT studies on the mechanism of veratryl alcohol oxidation catalyzed by Cuâ€“phen complexes. RSC Advances, 2014, 4, 30558-30565.	3.6	4
33	Europiumâ€linked structures and electronic properties of nanosize semiconductor <scp>EuSi_n⁰</scp>^{/â^'} (n = 11â€18) clusters. International Journal of Quantum Chemistry, 2021, 121, e26457.	2.0	4
34	Unraveling the Mechanism of Aerobic Alcohol Oxidation by a Cu/pytl-Î²-Cyclodextrin/TEMPO Catalytic System under Air in Neat Water. Inorganic Chemistry, 2021, 60, 14132-14141.	4.0	4
35	Mechanistic Insight into the 2Â° Alcohol Oxidation Mediated by an Efficient CuI/L-Proline-TEMPO Catalystâ€”A Density Functional Theory Study. Catalysts, 2017, 7, 264.	3.5	3
36	Mechanism of Aerobic Alcohol Oxidation Mediated by Waterâ€Soluble Cu^{II}â€TEMPO Catalyst in Water: A Density Functional Theory Study. ChemistrySelect, 2018, 3, 1268-1274.	1.5	3

#	Article	IF	Citations
37	DFT Studies on the Mechanism of Alcohol Oxidation Catalyzed by the Ni^{III}/bipy Complex. European Journal of Inorganic Chemistry, 2012, 2012, 2353-2358.	2.0	1
38	Theoretical study on the two-dimensional bis(iminothiolato)rhodium as oxygen reduction reaction catalyst. Molecular Physics, 2021, 119, e1817593.	1.7	0
39	First-principles calculations on electronic structures of Zn adsorbed on the anatase TiO2 (101) surface having oxygen vacancy and hydroxyl groups. Wuli Xuebao/Acta Physica Sinica, 2013, 62, 187101.	0.5	0