Xiang Zhang

List of Publications by Year
in descending order

33 papers	232 citations	1040056 9 h-index	1058476 14 g-index
33 all docs	33 docs citations	33 times ranked	324 citing authors

#	Article	IF	Citations
1	A new look at the essence of the formation of trigonal planar coordination of the central N and O atoms. Structural Chemistry, 2020, 31, 541-546.	2.0	0
2	1,2,4-Triazolato paddlewheel dibismuth complexes with very short Bi(ii)â€“Bi(ii) bonds: bismuth(iii) oxidation of 1,2,4-triazolato anions into neutral N-1,2,4-triazolyl radicals. Dalton Transactions, 2020, 49, 15190-15194.	3.3	1
3	Mechanistic Insights into the Chemoâ€Selective Dehydrogenative Silylation of Alkenes Catalyzed by Bis(imino)pyridine Cobalt Complex from DFT Computations. ChemCatChem, 2020, 12, 3890-3899.	3.7	2
4	A theoretical elucidation for the formation of unusual zwitterionic sandwich and terminal ruthenium complexes. Journal of Physical Organic Chemistry, 2020, 33, e4070.	1.9	0
5	Computational Insight into the Mechanism of Ruthenium(II)-Catalyzed Î±-Alkylation of Arylmethyl Nitriles Using Alcohols. Journal of Physical Chemistry A, 2019, 123, 10263-10272.	2.5	2
6	Molecular and dissociated adsorption of hydrogen on TiC6H6. International Journal of Hydrogen Energy, 2019, 44, 25800-25808.	7.1	8
7	Linear complex HC C-TMH (TM=Scâ€“Ni): A simple and efficient adsorbent for hydrogen molecules. International Journal of Hydrogen Energy, 2019, 44, 18145-18152.	7.1	8
8	Mechanisms and Activity of 1â€Phenylethanol Dehydrogenation Catalyzed by Bifunctional NHCâ€Ir^{III} Complex. European Journal of Organic Chemistry, 2019, 2019, 3929-3936.	2.4	4
9	Exploring the mechanism of alkene hydrogenation catalyzed by defined iron complex from DFT computation. Journal of Molecular Modeling, 2019, 25, 61.	1.8	3
10	Adsorption of multiple H2 molecules on the complex TiC6H6: An unusual combination of chemisorption and physisorption. Energy, 2019, 171, 315-325.	8.8	22
11	Theoretical elucidation on the mechanism of 1Hâ€1,2,4â€diazaphospholes synthesis from 1,3â€bis (amino)â€2â€phosphaallyl chlorides with hydrazine. Journal of Physical Organic Chemistry, 2019, 32, e3899.	1.9	2
12			

#	Article	IF	Citations
19	Mechanism for covalent dimerization of pyridine: [4+2] dimerization, an MP2 investigation. Chemical Physics Letters, 2016, 644, 132-137.	2.6	2
20	Theoretical study on the reaction of <mml:math altimg="si2.gif" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd" xmlns:ce="http://www.elsevier.com/xml/common/dtd" xmlns:xlink="http://www.w3.org/1999/xlink" xmlns:cals="http://www.elsevier.com/xml/common/cals/dtd">Chemi	2.6	1
21	A fluorescence onâ€“off sensor for Cu²⁺and its resultant complex as an offâ€“on sensor for Cr³⁺in aqueous media. RSC Advances, 2015, 5, 74629-74637.	3.6	21
22	Paddlewheel 1,2,4-diazaphospholide dibismuthanes with very short bismuthâ€“bismuth single bonds. Chemical Communications, 2015, 51, 16184-16187.	4.1	23
23	Mechanism for covalence bond benzene dimers formation: A DFT and MP2 investigation. Chemical Physics Letters, 2014, 610-611, 192-197.	2.6	5
24	The substitution reaction of (CNC)Feâ^'2N2 with CO. Journal of Molecular Modeling, 2013, 19, 2625-2633.	1.8	2
25	Direct ab initio study on the rate constants of radical C2(A3Îu)â€‰+â€‰C3H8 reaction. Journal of Molecular Modeling, 2013, 19, 1009-1018.	1.8	0
26	Mechanism Study of C₄H(X²â^⁺)+H₂Reaction by DirectAb InitioMethods. Acta Chimica Sinica, 2013, 71, 743.	1.4	4
27	Directab initiodynamics study of rate constants and kinetic isotope effects for C₂(A³Î_u)â€‰+â€‰CH₃OH reaction. Molecular Physics, 2012, 110, 2205-2217.	1.7	0
28	Direct ab initio dynamics study of the reaction of C₂(A³Î_u) with CH₄. International Journal of Quantum Chemistry, 2012, 112, 1078-1085.	2.0	10
29	Direct Ab Initio Dynamics Study of Radical C₄H (XÌƒ²Î£⁺) + CH₄ Reaction. Journal of Physical Chemistry A, 2011, 115, 3576-3582.	2.5	10
30	Direct ab initio dynamics study of the reaction of C2(A3Îu) radical with C2H6. Chemical Physics Letters, 2011, 503, 210-214.	2.6	7
31	Theoretical study on electronic structure of (CNC)Fe_2N₂ and its N₂ elimination mechanism. International Journal of Quantum Chemistry, 2010, 110, 1880-1889.	2.0	2
32	Theoretical Elucidation of the Platinum-Mediated Arene Câ^'H Activation Reactions. Organometallics, 2007, 26, 2203-2210.	2.3	16
33	Calculations of the geometries, electronic structures and nonlinear second-order optical susceptibilities of spiroannelated quinone-type methanofullerenes. Theoretical Chemistry Accounts, 2001, 106, 241-250.	1.4	9