Richard Tia

List of Publications by Year
in descending order

65	614	566801 15	713013 21
papers	citations	h-index	g-index

67	67	67	384
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A density functional theory study of the reactions of furans with substituted alkynes to form oxanorbornadienes and subsequent [4â€‰+â€‰2] and [2â€‰+â€‰2â€‰+â€‰2] addition reactions. Journal of Physical Organic Chemistry, 2022, 35, e4281.	0.9	1
2	A DFT Mechanistic Study on Base-Catalyzed Cleavage of the Î²-O-4 Ether Linkage in Lignin: Implications for Selective Lignin Depolymerization. Frontiers in Chemistry, 2022, 10, 793759.	1.8	1
3	First-principles DFT insights into the mechanisms of CO2 reduction to CO on Fe (100)-Ni bimetals. Theoretical Chemistry Accounts, 2022, 141, .	0.5	2
4	A DFT study of the oxygen reduction reaction mechanism on be doped graphene. Chemical Papers, 2022, 76, 4471-4480.	1.0	1
5	Computational exploration of the 1,3â€dipolar cycloaddition reaction of 7â€isopropylidenebenzonorbornadiene with nitrile oxide and cyclic nitrone derivatives. Journal of Physical Organic Chemistry, 2021, 34, e4174.	0.9	6
6	The 1,3-dipolar cycloaddition of adamantine-derived nitrones with maleimides: A computational study. Computational and Theoretical Chemistry, 2021, 1195, 113099.	1.1	4
7	Regioâ€ enantioâ€ periâ€ and stereoâ€selectivities of the reactions of fiveâ€membered cyclodiene derivatives with itaconic anhydride toward the formation of norbornene lactones. Journal of Physical Organic Chemistry, 2021, 34, e4132.	0.9	3
8	Mechanism of Guaiacol Hydrodeoxygenation on Cu (111): Insights from Density Functional Theory Studies. Catalysts, 2021, 11, 523.	1.6	5
9	A DFT mechanistic study on oxidative dehydrogenative Dielsâ€“Alder reaction of alkylbenzenes. Journal of Molecular Graphics and Modelling, 2021, 104, 107839.	1.3	3
10	Regioâ€ stereoâ€ and siteâ€selectivities of 1,3â€dipolar Cycloaddition reaction of benzonitrile oxide with unsymmetrically substituted norbornenes and norbornadienes: A computational study. Journal of Physical Organic Chemistry, 2021, 34, e4259.	0.9	4
11	Ferrocenylimine Palladium (II) Complexes: Synthesis, Characterization and Application in Mizoroki-Heck and Suzuki-Miyaura Cross-Coupling Reactions. Catalysts, 2021, 11, 755.	1.6	5
12	Quantum chemical investigation of the formation of spiroheterocyclic compounds via the (3Â+ 2) cycloaddition reaction of 1-methyl-3-(2,2,2-trifluoroethylidene) pyrrolidin-2-one with diazomethane and nitrone derivatives. Tetrahedron, 2021, 94, 132306.	1.0	4
13	Investigating the site-, regio-, and stereo-selectivities of the reactions between organic azide and 7-heteronorbornadiene: a DFT mechanistic study. Journal of Molecular Modeling, 2021, 27, 248.	0.8	4
14	Exploring the chemo-, regio-, and stereoselectivities of the (3â€‰+â€‰2) cycloaddition reaction of 5,5-dimethyl-3-methylene-2-pyrrolidinone with C,N-diarylnitrones and nitrile oxide derivatives: a DFT study. Journal of Molecular Modeling, 2021, 27, 287.	0.8	2
15	Does the reaction of nitrone derivatives with allenoates proceed by an initial (3 + 2) cycloaddition or O-Nucleophilic addition? A quantum chemical investigation. Journal of Molecular Graphics and Modelling, 2021, 109, 108036.	1.3	1
16	A DFT study of the double (3 + 2) cycloaddition of nitrile oxides and allenoates for the formation of spirobiisoxazolines. Journal of Molecular Graphics and Modelling, 2021, 109, 108033.	1.3	3
17	Theoretical investigation of the regio-, enantio-, and stereo-selectivities of the (3â€‰+â€‰2) cycloaddition reactions of N-vinylindoles with nitrones and nitrile oxides. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	0
18	The mechanisms of gallium-catalysed skeletal rearrangement of 1,6-enynes â€“ Insights from quantum mechanical computations. Journal of Molecular Graphics and Modelling, 2020, 94, 107476.	1.3	7

#	Article	IF	Citations
19	Site-, enantio- and stereo-selectivities of the 1,3-dipolar cycloaddition reactions of oxanorbornadiene with C,N-disubstituted nitrones and dimethyl nitrilimines: a DFT mechanistic study. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	22
20	Computational study on the mechanism of the reaction of benzenesulfonyl azides with oxabicyclic alkenes. Journal of Molecular Modeling, 2020, 26, 314.	0.8	4
21	Influence of Topology and BrÃ¸nsted Acid Site Presence on Methanol Diffusion in Zeolites Beta and MFI. Catalysts, 2020, 10, 1342.	1.6	11
22	A DFT mechanistic study on [4Â+Â3] cycloaddition reactions of oxyallyl cations and five-membered cyclopentadiene derivatives. Tetrahedron, 2020, 76, 131422.	1.0	4
23	1,3-Dipolar cycloaddition reaction of indoles with tosyl azide, subsequent dehydroaromatization and ring-opening cascade: a computational study. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	10
24	(3Â+ 2) cycloaddition reaction of 7-isopropylidenebenzonorbornadiene and diazomethane derivatives: A theoretical study. Journal of Molecular Graphics and Modelling, 2020, 101, 107713.	1.3	10
25	Catalytic isomerizationâ€“hydroformylation of olefins by rhodium salicylaldimine pre-catalysts. New Journal of Chemistry, 2020, 44, 8751-8762.	1.4	6
26	Mechanistic study of the tandem intramolecular (4 +â€‰2)/intermolecular (3 +â€‰2) cycloaddition reactions for the formation of polyazaâ€•and polyisoxazolidineâ€steroids. Journal of Heterocyclic Chemistry, 2020, 57, 1748-1758.	1.4	16
27	Investigating the regio-, stereo-, and enantio-selectivities of the 1,3-dipolar cycloaddition reaction of C-cyclopropyl-N-phenylnitrone derivatives and benzylidenecyclopropane derivatives: A DFT study. Journal of Molecular Graphics and Modelling, 2020, 100, 107672.	1.3	11
28	Permanganyl chloride-mediated oxidation of tetramethylethylene: A density functional theory study. Journal of Molecular Graphics and Modelling, 2020, 98, 107616.	1.3	3
29	Peri-, Chemo-, Regio-, Stereo- and Enantio-Selectivities of 1,3-dipolar cycloaddition reaction of C,N-Disubstituted nitrones with disubstituted 4-methylene-1,3-oxazol-5(4H)- one: A quantum mechanical study. Journal of Molecular Graphics and Modelling, 2020, 97, 107542.	1.3	17
30	DFT mechanistic studies on the regio-, stereo-, and enantio-selectivity of 1,3 dipolar cycloadditions of quinolinium imides with olefins, maleimides, and benzynes for the synthesis of fused N,Nâ€²-heterocycles. Journal of Molecular Modeling, 2020, 26, 36.	0.8	2
31	A DFT investigation of the mechanisms of CO2 and CO methanation on Fe (111). Materials for Renewable and Sustainable Energy, 2020, 9, 1.	1.5	7
32	1, 3-Dipolar cycloaddition reactions of selected 1,3-dipoles with 7-isopropylidenenorbornadiene and follow-up thermolytic cleavage: A computational study. Journal of Molecular Graphics and Modelling, 2019, 92, 267-279.	1.3	24
33	Quantum chemical studies on the mechanistic aspects of tandem sequential cycloaddition reactions of cyclooctatetraene with ester and nitrones. Journal of Molecular Graphics and Modelling, 2019, 92, 17-31.	1.3	30
34	Hydrogenation of carbon dioxide to formate by Î±-diimine RuII, RhIII, IrIII complexes as catalyst precursors. Journal of Organometallic Chemistry, 2019, 899, 120892.	0.8	17
35	Mechanistic studies on tandem cascade [4Â+ 2]/ [3Â+ 2] cycloaddition of 1,3,4-oxadiazoles with olefins. Journal of Molecular Graphics and Modelling, 2019, 93, 107452.	1.3	22
36	DFT mechanistic study on tandem sequential [4Â+Â2]/[3Â+Â2] addition reaction of cyclooctatetraene with functionalized acetylenes and nitrile imines. Journal of Physical Organic Chemistry, 2019, 32, e3992.	0.9	35

#	Article	IF	Citations
37	Computational studies on [4â€‰+â€‰2] / [3â€‰+â€‰2] tandem sequential cycloaddition reactions of functionalized acetylenes with cyclopentadiene and diazoalkane for the formation of norbornene pyrazolines. Journal of Molecular Modeling, 2019, 25, 168.	0.8	32
38	Hydrazine adsorption on perfect and defective fcc nickel (100), (110) and (111) surfaces: A dispersion corrected DFT-D2 study. Applied Surface Science, 2019, 480, 1014-1024.	3.1	13
39	Trapping of 1,2-cyclohexadiene: A DFT mechanistic study on the reaction of 1,2-cyclohexadiene with olefins and nitrones. Journal of Molecular Graphics and Modelling, 2018, 81, 1-13.	1.3	4
40	Computational study on the mechanism of transition metal-catalyzed formation of highly substituted furo [3,4-d] [1,2] oxazines. Journal of Theoretical and Computational Chemistry, 2018, 17, 1850011.	1.8	3
41	Density functional theory studies onÂthe generation of trimethylenemethanes from the ring opening of dialkoxymethylenecyclopropanes and methylenecyclopropanethioacetals and follow-up reactions. Journal of Molecular Modeling, 2018, 24, 24.	0.8	3
42	Ab initio investigation of O₂ adsorption on Ca-doped LaMnO₃ cathodes in solid oxide fuel cells. Physical Chemistry Chemical Physics, 2018, 20, 28685-28698.	1.3	9
43	A DFT mechanistic study of the generation of azomethine ylides from the ring-opening reactions of stabilized aziridines and follow-up 1,3-dipolar cycloaddition reactions with acetaldehyde. Computational and Theoretical Chemistry, 2018, 1144, 38-49.	1.1	8
44	Diels-Alder cycloaddition versus ring-opening esterification: A computational study of the mechanism of formation of oxa-norbonene lactones from the reaction of furfuryl alcohol and itaconic anhydride. Computational and Theoretical Chemistry, 2018, 1138, 7-14.	1.1	7
45	Water-soluble SNS cationic palladium(II) complexes and their Suzukiâ€“Miyaura cross-coupling reactions in aqueous medium. Beilstein Journal of Organic Chemistry, 2018, 14, 1859-1870.	1.3	23
46	A DFT+U investigation of hydrogen adsorption on the LaFeO₃(010) surface. Physical Chemistry Chemical Physics, 2017, 19, 7399-7409.	1.3	28
47	Effect of nickel monolayer deposition on the structural and electronic properties of the low miller indices of (bcc) iron: A DFT study. Applied Surface Science, 2017, 400, 293-303.	3.1	12
48	CO₂ activation and dissociation on the low miller index surfaces of pure and Ni-coated iron metal: a DFT study. Physical Chemistry Chemical Physics, 2017, 19, 19478-19486.	1.3	18
49	[3 + 2] versus [2 + 2] Addition: A Density Functional Theory Study on the Mechanistic Aspects of Transition Metal-Assisted Formation of 1,2-Dinitrosoalkanes. Journal of Chemistry, 2016, 2016, 1-10.	0.9	16
50	1,3-Dipolar [3Â+Â2] cycloaddition reactions of N,C,C-trisubstituted nitrones with ring-acceptor methylenecyclopropanes: a computational study. SpringerPlus, 2016, 5, 2072.	1.2	6
51	A quantum chemical study of the mechanisms of olefin addition to group 9 transition metal dioxo compounds. SpringerPlus, 2016, 5, 867.	1.2	2
52	Mechanistic studies on Diels-Alder [4Â+Â2] cycloaddition reactions of Î±,Î²-substituted cyclobutenones: Role of substituents in regio- and stereoselectivity. Tetrahedron, 2016, 72, 8261-8273.	1.0	7
53	A computational study of the addition of ReO3L (LÂ=ÂClâ¯, CH3, OCH3 and Cp) to ethenone. SpringerPlus, 2016, 5, 354.	1.2	1
54	Quantum chemical study of the mechanisms of oxidation of ethylene by Molybdyl and Tungstyl Chloride. Journal of Chemical Sciences, 2016, 128, 707-718.	0.7	2

#	Article	IF	Citations
55	A density functional theory study of arsenic immobilization by the Al(<scp>iii</scp>)-modified zeolite clinoptilolite. Physical Chemistry Chemical Physics, 2016, 18, 11297-11305.	1.3	14
56	Exploring the peri-, chemo-, and regioselectivity of addition of technetium metal oxides of the type TcO₃L (L = Cl^{â€“}, O^{â€“}, OCH₃, CH₃) to substituted ketenes: a DFT computational study. Canadian Journal of Chemistry, 2016, 94, 523-532.	0.6	0
57	Exploring the peri-, chemo-, and regio-selectivity of addition of manganese metal oxides MnO3L (L =) Tj ETQq1 1 0.784314 rgBT /Over 57-66.	1.2	2
58	A density functional theory study of the mechanisms of addition of transition metal oxides ReO₃L(L = Cl⁻,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 substituted ketenes. Journal of Theoretical and Computational Chemistry, 2015, 14, 1550035.	1.8	4
59	A density functional theory study of the mechanisms of oxidation of ethylene by rhenium oxide complexes. Dalton Transactions, 2013, 42, 10885.	1.6	13
60	A density functional theory study of the mechanisms of oxidation of ethylene by technetium oxo complexes. Computational and Theoretical Chemistry, 2013, 1009, 70-80.	1.1	18
61	A theoretical study of the mechanisms of oxidation of ethylene by manganese oxo complexes. Dalton Transactions, 2013, 42, 14411.	1.6	15
62	Computational studies of the mechanistic aspects of olefin metathesis reactions involving metal oxo-alkylidene complexes. Computational and Theoretical Chemistry, 2011, 971, 8-18.	1.1	9
63	[3+2] Versus [2+2] addition of metal oxides across CC bonds: A theoretical study of the mechanisms of oxidation of ethylene by osmium oxide complexes. Computational and Theoretical Chemistry, 2011, 977, 140-147.	1.1	17
64	Density functional theory studies of the mechanistic aspects of olefin metathesis reactions. Dalton Transactions, 2010, 39, 7575.	1.6	8
65	Density Functional Theory Study of the Mechanisms of Oxidation of Ethylene by Chromyl Chloride. Inorganic Chemistry, 2009, 48, 11434-11443.	1.9	13