Qingxi Meng

List of Publications by Year
in descending order

39 papers	222 citations	1163117 8 h-index	1281871 11 g-index
39 all docs	39 docs citations	39 times ranked	221 citing authors

#	Article	IF	Citations
1	Density functional studies on copper-catalyzed asymmetric cyclopropanation of diazoacetate with alkene. Computational and Theoretical Chemistry, 2004, 711, 193-199.	1.5	21
2	What accounts for the color purity of tetradentate Pt complexes? A computational analysis. Physical Chemistry Chemical Physics, 2019, 21, 8073-8080.	2.8	15
3	Small substituent groups as geometric controllers for tridentate platinum(<scp>ii</scp>) complexes to effectively suppress non-radiative decay processes. Physical Chemistry Chemical Physics, 2019, 21, 2764-2770.	2.8	14
4	Theoretical insights of copper(I) carbenes. Computational and Theoretical Chemistry, 2006, 765, 13-20.	1.5	13
5	Density functional computations of the cyclopropanation of ethene catalyzed by iron (II) carbene complexes Cp(CO)(L)Feï£¾CHR, L = CO, PMe₃, R = Me, OMe, ph, CO₂Me. International Journal of Quantum Chemistry, 2008, 108, 945-953.	2.0	12
6	Mechanism of intermolecular hydroacylation of vinylsilanes catalyzed by a rhodium(I) olefin complex: a DFT study. Journal of Molecular Modeling, 2012, 18, 1229-1239.	1.8	9
7	Lysine Ethylation by Histone Lysine Methyltransferases. ChemBioChem, 2020, 21, 392-400.	2.6	9
8	Theoretical Insight into Ni(0)-Catalyzed Hydroarylation of Alkenes and Arylboronic Acids. Journal of Organic Chemistry, 2020, 85, 13264-13271.	3.2	9
9	Ruthenium hydride-catalyzed regioselective addition of benzaldehyde to dienes leading to Î²,Î³-unsaturated ketones: a DFT study. Journal of Molecular Modeling, 2012, 18, 4955-4963.	1.8	8
10	Theoretical investigation of Ni(PMe3)4-catalyzed intermolecular hydroacylation of alkynes with benzaldehydes. Transition Metal Chemistry, 2011, 36, 793-799.	1.4	7
11	Mechanism for Co(dppp)-catalyzed regioselective intermolecular hydroacylation of 1,3-dienes and benzaldehydes: Insights from density functional calculations. Journal of Organometallic Chemistry, 2018, 868, 102-111.	1.8	7
12	Theoretical insights of iron(II)â€“carbene complexes Cp(CO)(L)FeCHR, L=CO, PMe3. Computational and Theoretical Chemistry, 2007, 815, 157-163.	1.5	6
13	Density functional computations of Rh(I)-catalysed hydroacylation of acetic aldehyde and ethene. Molecular Simulation, 2008, 34, 515-523.	2.0	6
14	Theoretical studies of ruthenium hydride-catalyzed addition reactions of benzaldehydes to isoprenes leading to Î²,Î³-unsaturated ketones: The role of the ligands hydride, carbonyl, chloride, and triphenylphosphine of the catalyst. Journal of Organometallic Chemistry, 2014, 753, 1-8.	1.8	6
15	Theoretical studies of cobalt(I)-catalyzed hydroacylation of vinylsilanes and alkyl aldehydes. Journal of Physical Organic Chemistry, 2015, 28, 431-436.	1.9	6
16	Mechanisms and reactivity differences for the cobalt-catalyzed enantioselective intramolecular hydroacylation of ketones and alkenes: insights from density functional calculations. Journal of Molecular Modeling, 2016, 22, 60.	1.8	6
17	Mechanisms for nickel(0)/N-heterocyclic carbene-catalyzed intramolecular alkene hydroacylation: insights from a DFT study. Journal of Molecular Modeling, 2017, 23, 11.	1.8	6
18	Density functional computations of enantioselective alkynylation of aldehyde catalyzed by chiral zinc(II)-complexes. Journal of Molecular Modeling, 2006, 12, 494-502.	1.8	5

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19	Density functional computations of alkynylation of nitrones catalyzed by chiral zinc(II)-complexes. Structural Chemistry, 2009, 20, 129-137.	2.0	5
20	Theoretical investigation of Co(0)-catalyzed intramolecular hydroacylation of 4-pentenal. Journal of Molecular Modeling, 2013, 19, 2225-2234.	1.8	5
21	Nickel/zinc-catalyzed decarbonylative addition of anhydrides to alkynes: A DFT study. Journal of Molecular Modeling, 2013, 19, 4545-4554.	1.8	5
22	Theoretical studies of palladium-catalyzed cycloaddition of alkynyl aryl ethers and alkynes. Journal of Molecular Modeling, 2014, 20, 2514.	1.8	5
23	Strategy Used to Control the Mechanism of Homogeneous Alkyne/Olefin Hydrogenation: AIMD Simulations and DFT Calculations. Journal of Organic Chemistry, 2020, 85, 11626-11634.	3.2	5
24	Density function studies on the PtCl2-catalyzed asymmetric cycloisomerization reaction of hydroxylated enynes. International Journal of Quantum Chemistry, 2006, 106, 1569-1579.	2.0	4
25	Density functional computations of Rh(I)-catalysed hydroacylation and hydrogenation of ethene using formic acid. Molecular Simulation, 2009, 35, 419-427.	2.0	4
26	DENSITY FUNCTIONAL COMPUTATIONS OFRh(I)-CATALYZED HYDROACYLATION OF ETHENE OR ETHYNE. Journal of Theoretical and Computational Chemistry, 2008, 07, 1041-1053.	1.8	3
27	Density functional studies on copper-catalysed asymmetric aziridination of diazoacetate with imines. Molecular Simulation, 2010, 36, 15-25.	2.0	3
28	Substituent effect and ligand exchange control the reactivity in ruthenium(II)-catalyzed hydroacylation of isoprenes and aldehydes â€– A DFT study. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650019.	1.8	3
29	Mechanism for ruthenium hydride-catalyzed regioselective hydroacylation of enones and aldehydes to give 1,3-diketones: Insights from density functional calculations. Molecular Catalysis, 2017, 433, 55-61.	2.0	3
30	Theoretical studies on the Mo-catalyzed asymmetric intramolecular Pauson-Khand-type [2â€‰+â€‰2â€‰+â€‰1] cycloadditions of 3-allyloxy-1-propynylphosphonates. Journal of Molecular Modeling, 2012, 18, 3489-3499.	1.8	2
31	Mechanistic study on Mo(CO)₆â€catalyzed intramolecular [2â€‰+â€‰2] or [2â€‰+â€‰2â€‰+â€‰1] cycloaddition reaction of 5â€allenylâ€1â€ynes. Journal of Physical Organic Chemistry, 2012, 25, 21-31.	1.9	2
32	Density functional calculations for Rh(I)â€catalyzed Câ€“C bond activation of siloxyvinylcyclopropanes and diazoesters. Applied Organometallic Chemistry, 2019, 33, e4869.	3.5	2
33	Theoretical Study of Nâ€“H Ïƒ-Bond Activation by Nickel(0) Complex: Reaction Mechanism, Electronic Processes, and Prediction of Better Ligand. Inorganic Chemistry, 2022, 61, 8715-8728.	4.0	2
34	Density functional computations of alkynylation of ethanimine catalyzed by chiral zinc(II)â€complexes. International Journal of Quantum Chemistry, 2008, 108, 362-369.	2.0	1
35	Theoretical studies of nickel-catalyzed ring-opening hydroacylation of methylenecyclopropanes and benzaldehydes. Journal of Molecular Modeling, 2015, 21, 203.	1.8	1
36	Theoretical Studies for Switching Regioselectivity in Ruthenium Hydrideâ€Catalyzed Alkyne Hydroacylation. ChemistrySelect, 2017, 2, 2858-2865.	1.5	1

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37	Density Functional Computations for Co(I)â€Catalyzed Intermolecular Hydroacylation of Benzaldehydes. ChemistrySelect, 2019, 4, 11315-11320.	1.5	1
38	Mechanism of rhodiumâ€catalyzed hydroacylation of propylene using formaldehyde: A computational study. International Journal of Quantum Chemistry, 2010, 110, 850-859.	2.0	0
39	Phosphine ligand-coated Cu nanoparticle-catalyzed selective semihydrogenation of alkynes: electronic or hindrance effects of the ligand?. Physical Chemistry Chemical Physics, 2020, 22, 16905-16913.	2.8	0