

# Qingxi Meng

## List of Publications by Year in descending order

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papers

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#	ARTICLE	IF	CITATIONS
1	Theoretical Study of $\sigma$ -H $\pi$ -Bond Activation by Nickel(0) Complex: Reaction Mechanism, Electronic Processes, and Prediction of Better Ligand. <i>Inorganic Chemistry</i> , 2022, 61, 8715-8728.	4.0	2
2	Lysine Ethylation by Histone Lysine Methyltransferases. <i>ChemBioChem</i> , 2020, 21, 392-400.	2.6	9
3	Theoretical Insight into Ni(0)-Catalyzed Hydroarylation of Alkenes and Arylboronic Acids. <i>Journal of Organic Chemistry</i> , 2020, 85, 13264-13271.	3.2	9
4	Strategy Used to Control the Mechanism of Homogeneous Alkyne/Olefin Hydrogenation: AIMD Simulations and DFT Calculations. <i>Journal of Organic Chemistry</i> , 2020, 85, 11626-11634.	3.2	5
5	Phosphine ligand-coated Cu nanoparticle-catalyzed selective semihydrogenation of alkynes: electronic or hindrance effects of the ligand?. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16905-16913.	2.8	0
6	Small substituent groups as geometric controllers for tridentate platinum( $\sigma$ -Cp) complexes to effectively suppress non-radiative decay processes. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 2764-2770.	2.8	14
7	Density Functional Computations for Co(I)-Catalyzed Intermolecular Hydroacylation of Benzaldehydes. <i>ChemistrySelect</i> , 2019, 4, 11315-11320.	1.5	1
8	Density functional calculations for Rh(I)-catalyzed C=C bond activation of siloxyvinylcyclopropanes and diazoesters. <i>Applied Organometallic Chemistry</i> , 2019, 33, e4869.	3.5	2
9	What accounts for the color purity of tetradentate Pt complexes? A computational analysis. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8073-8080.	2.8	15
10	Mechanism for Co(dppp)-catalyzed regioselective intermolecular hydroacylation of 1,3-dienes and benzaldehydes: Insights from density functional calculations. <i>Journal of Organometallic Chemistry</i> , 2018, 868, 102-111.	1.8	7
11	Mechanisms for nickel(0)/N-heterocyclic carbene-catalyzed intramolecular alkene hydroacylation: insights from a DFT study. <i>Journal of Molecular Modeling</i> , 2017, 23, 11.	1.8	6
12	Mechanism for ruthenium hydride-catalyzed regioselective hydroacylation of enones and aldehydes to give 1,3-diketones: Insights from density functional calculations. <i>Molecular Catalysis</i> , 2017, 433, 55-61.	2.0	3
13	Theoretical Studies for Switching Regioselectivity in Ruthenium Hydride-Catalyzed Alkyne Hydroacylation. <i>ChemistrySelect</i> , 2017, 2, 2858-2865.	1.5	1
14	Substituent effect and ligand exchange control the reactivity in ruthenium(II)-catalyzed hydroacylation of isoprenes and aldehydes – A DFT study. <i>Journal of Theoretical and Computational Chemistry</i> , 2016, 15, 1650019.	1.8	3
15	Mechanisms and reactivity differences for the cobalt-catalyzed enantioselective intramolecular hydroacylation of ketones and alkenes: insights from density functional calculations. <i>Journal of Molecular Modeling</i> , 2016, 22, 60.	1.8	6
16	Theoretical studies of cobalt(I)-catalyzed hydroacylation of vinylsilanes and alkyl aldehydes. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 431-436.	1.9	6
17	Theoretical studies of nickel-catalyzed ring-opening hydroacylation of methylenecyclopropanes and benzaldehydes. <i>Journal of Molecular Modeling</i> , 2015, 21, 203.	1.8	1
18	Theoretical studies of ruthenium hydride-catalyzed addition reactions of benzaldehydes to isoprenes leading to $\beta,\gamma$ -unsaturated ketones: The role of the ligands hydride, carbonyl, chloride, and triphenylphosphine of the catalyst. <i>Journal of Organometallic Chemistry</i> , 2014, 753, 1-8.	1.8	6

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19	Theoretical studies of palladium-catalyzed cycloaddition of alkynyl aryl ethers and alkynes. Journal of Molecular Modeling, 2014, 20, 2514.	1.8	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 on the Mo-catalyzed asymmetric intramolecular Pauson-Khand-type [2+2+1] cycloadditions of 3-allyloxy-1-propynylphosphonates. Journal of Molecular Modeling, 2012, 18, 3489-3499.	1.8	2
23	Ruthenium hydride-catalyzed regioselective addition of benzaldehyde to dienes leading to $\eta^2, \eta^3$ -unsaturated ketones: a DFT study. Journal of Molecular Modeling, 2012, 18, 4955-4963.	1.8	8
24	Mechanistic study on Mo(CO) <sub>6</sub> -catalyzed intramolecular [2+2] or [2+2+1] cycloaddition reaction of allenylalkynes. Journal of Physical Organic Chemistry, 2012, 25, 21-31.	1.9	2
25	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
26	Theoretical investigation of Ni(PMe <sub>3</sub> ) <sub>4</sub> -catalyzed intermolecular hydroacylation of alkynes with benzaldehydes. Transition Metal Chemistry, 2011, 36, 793-799.	1.4	7
27	Mechanism of rhodium-catalyzed hydroacylation of propylene using formaldehyde: A computational study. International Journal of Quantum Chemistry, 2010, 110, 850-859.	2.0	0
28	Density functional studies on copper-catalysed asymmetric aziridination of diazoacetate with imines. Molecular Simulation, 2010, 36, 15-25.	2.0	3
29	Density functional computations of Rh(I)-catalysed hydroacylation and hydrogenation of ethene using formic acid. Molecular Simulation, 2009, 35, 419-427.	2.0	4
30	Density functional computations of alkynylation of nitrones catalyzed by chiral zinc(II)-complexes. Structural Chemistry, 2009, 20, 129-137.	2.0	5
31	Density functional computations of alkynylation of ethanimine catalyzed by chiral zinc(II)-complexes. International Journal of Quantum Chemistry, 2008, 108, 362-369.	2.0	1
32	Density functional computations of the cyclopropanation of ethene catalyzed by iron (II) carbene complexes Cp(CO)(L)FeCHR, L = CO, PMe <sub>3</sub> , R = Me, OMe, ph, CO <sub>2</sub> Me. International Journal of Quantum Chemistry, 2008, 108, 945-953.	2.0	12
33	DENSITY FUNCTIONAL COMPUTATIONS OF Rh(I)-CATALYZED HYDROACYLATION OF ETHENE OR ETHYNE. Journal of Theoretical and Computational Chemistry, 2008, 07, 1041-1053.	1.8	3
34	Density functional computations of Rh(I)-catalysed hydroacylation of acetic aldehyde and ethene. Molecular Simulation, 2008, 34, 515-523.	2.0	6
35	Theoretical insights of iron(II)-carbene complexes Cp(CO)(L)FeCHR, L=CO, PMe <sub>3</sub> . Computational and Theoretical Chemistry, 2007, 815, 157-163.	1.5	6
36	Density function studies on the PtCl <sub>2</sub> -catalyzed asymmetric cycloisomerization reaction of hydroxylated enynes. International Journal of Quantum Chemistry, 2006, 106, 1569-1579.	2.0	4

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37	Theoretical insights of copper(I) carbenes. Computational and Theoretical Chemistry, 2006, 765, 13-20.	1.5	13
38	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
39	Density functional studies on copper-catalyzed asymmetric cyclopropanation of diazoacetate with alkene. Computational and Theoretical Chemistry, 2004, 711, 193-199.	1.5	21