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List of Publications by Year
in descending order

65 papers	1,271 citations	394421 19 h-index	377865 34 g-index
65 all docs	65 docs citations	65 times ranked	1692 citing authors

#	Article	IF	Citations
1	Hydroboration of CO₂ to Methyl Boronate Catalyzed by a Manganese Pincer Complex: Insights into the Reaction Mechanism and Ligand Effect. Inorganic Chemistry, 2022, 61, 5616-5625.	4.0	16
2	A theoretical study of asymmetric ketone hydrogenation catalyzed by Mn complexes: from the catalytic mechanism to the catalyst design. Physical Chemistry Chemical Physics, 2022, 24, 13365-13375.	2.8	8
3	A theoretical study on the hydrogenation of CO₂to methanol catalyzed by ruthenium pincer complexes. Dalton Transactions, 2022, 51, 10020-10028.	3.3	10
4	A theoretical study of the hydroboration of Î±,Î²-unsaturated carbonyl compounds catalyzed by a metal-free complex and subsequent Câ€“C coupling with acetonitrile. New Journal of Chemistry, 2021, 45, 14134-14140.	2.8	3
5	Mechanistic Understanding of Baseâ€Catalyzed Aldimine/Ketoamine Condensations: An Old Story and A New Model. Asian Journal of Organic Chemistry, 2021, 10, 634-641.	2.7	7
6	Using Bases as Initiators to Isomerize Allylic Alcohols: Insights from Density Functional Theory Studies. Journal of Physical Chemistry A, 2021, 125, 2316-2323.	2.5	1
7	Theoretical investigation of Prolylâ€Histidineâ€catalyzed intermolecular aldol reaction. Journal of Physical Organic Chemistry, 2021, 34, e4203.	1.9	0
8	Composition-tunable PtCu porous nanowires as highly active and durable catalyst for oxygen reduction reaction. International Journal of Hydrogen Energy, 2021, 46, 18284-18293.	7.1	18
9	Pt-Based Intermetallic Nanocrystals in Cathode Catalysts for Proton Exchange Membrane Fuel Cells: From Precise Synthesis to Oxygen Reduction Reaction Strategy. Catalysts, 2021, 11, 1050.	3.5	20
10	First-Principles Study on the Mechanism of Nitrobenzene Reduction to Aniline Catalyzed by a N-Doped Carbon-Supported Cobalt Single-Atom Catalyst. Journal of Physical Chemistry C, 2021, 125, 19171-19182.	3.1	15
11	Mechanism of the Zinc Dithiocarbamate-Activated Rubber Vulcanization Process: A Density Functional Theory Study. ACS Applied Polymer Materials, 2021, 3, 5188-5196.	4.4	16
12	Theoretical study on the mechanism of C N and C C coupling to form indole catalyzed by Pd(OAc)2. Molecular Catalysis, 2021, 515, 111895.	2.0	4
13	A phosphine-free Mn(<scp>i</scp>)-NNS catalyst for asymmetric transfer hydrogenation of acetophenone: a theoretical prediction. Dalton Transactions, 2021, 50, 14738-14744.	3.3	7
14	Hydrogenation of CO₂to methanol catalyzed by a manganese pincer complex: insights into the mechanism and solvent effect. Dalton Transactions, 2021, 50, 7348-7355.	3.3	19
15	The Role of AQ in the Regioselectivity of Strong Alkyl Câ€“O Bond Activation Catalyzed by Pd(OAc)₂: A Density Functional Theory Mechanistic Study. Inorganic Chemistry, 2021, 60, 17555-17564.	4.0	7
16	Effect of point defects on acetylene hydrogenation reaction over Ni(111) surface: a density functional theory study. Physical Chemistry Chemical Physics, 2021, 23, 27340-27347.	2.8	1
17	The reaction paths of CH₂O decomposition on CuO(111) surface: A DFT study. Journal of Physical Organic Chemistry, 2020, 33, e4017.	1.9	4
18	A mesoporous carbon-based catalyst derived from cobalt and boron co-doped melamine formaldehyde gel for oxygen reduction reaction. Electrochimica Acta, 2020, 333, 135560.	5.2	12

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19	Theoretical Studies on the Stability and Reactivity of the Metal-Doped CeO₂(100) Surface: Toward H₂ Dissociation and Oxygen Vacancy Formation. Langmuir, 2020, 36, 5891-5901.	3.5	42
20	Asymmetric Induction with a Chiral Amine Catalyzed by a Ru-PNP Pincer Complex: Insight from Theoretical Investigation. Inorganic Chemistry, 2020, 59, 8404-8411.	4.0	13
21	Transition-metal-free polycyclic indoline formation via a free radical pathway: a computational mechanistic study. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	3
22	pH-Dependent transfer hydrogenation or dihydrogen release catalyzed by a [(Î·6-arene)RuCl(Îº2-N,N-dmobpy)]+ complex: a DFT mechanistic understanding. RSC Advances, 2020, 10, 10411-10419.	3.6	7
23	Pt-based trimetallic nanocrystals with high proportions of M (M=Fe, Ni) metals for catalyzing oxygen reduction reaction. International Journal of Hydrogen Energy, 2020, 45, 16039-16048.	7.1	17
24	Theoretical Study on Nitrogenous Heterocyclic Assisted Aldimine Condensation. Acta Chimica Sinica, 2020, 78, 437.	1.4	7
25	Increasing the Activity and Selectivity of TiO₂-Supported Au Catalysts for Renewable Hydrogen Generation from Ethanol Photoreforming by Engineering Ti³⁺ Defects. ACS Sustainable Chemistry and Engineering, 2019, 7, 13856-13864.	6.7	57
26	Highly Efficient Lithium Recovery from Pre-Synthesized Chlorine-Ion-Intercalated LiAl-Layered Double Hydroxides via a Mild Solution Chemistry Process. Materials, 2019, 12, 1968.	2.9	19
27	Determination of boundary conditions for highly efficient separation of magnesium and lithium from salt lake brine by reaction-coupled separation technology. Separation and Purification Technology, 2019, 229, 115813.	7.9	34
28	Ruthenium-catalyzed deoxygenative hydroboration of carboxylic acids: a DFT mechanistic study. New Journal of Chemistry, 2019, 43, 11493-11496.	2.8	5
29	Inside Cover: A Computational Study on Iridiumâ€Catalyzed Production of Acetic Acid from Ethanol and Water Solution (Chin. J. Chem. 9/2019). Chinese Journal of Chemistry, 2019, 37, 862-862.	4.9	0
30	Theoretical study on the reaction mechanism and selectivity of acetylene semi-hydrogenation on Niâ€“Sn intermetallic catalysts. Physical Chemistry Chemical Physics, 2019, 21, 1384-1392.	2.8	10
31	A Computational Study on Iridiumâ€Catalyzed Production of Acetic Acid from Ethanol and Water Solution. Chinese Journal of Chemistry, 2019, 37, 883-886.	4.9	7
32	The reaction mechanism and selectivity of acetylene hydrogenation over Niâ€“Ga intermetallic compound catalysts: a density functional theory study. Dalton Transactions, 2018, 47, 4198-4208.	3.3	38
33	Energy-level dependent H 2 O 2 production on metal-free, carbon-content tunable carbon nitride photocatalysts. Journal of Energy Chemistry, 2018, 27, 343-350.	12.9	60
34	1,2 addition or cycloaddition of allenes by a dihafnium Î¼â^'Nitrido complex? A DFT study. Journal of Organometallic Chemistry, 2018, 874, 101-105.	1.8	1
35	Theoretical Study of the Histidine-catalyzed Asymmetric Aldol Reaction of Acetone and Benzaldehyde. Journal of Physical Chemistry A, 2018, 122, 7842-7851.	2.5	4
36	Structure Simulation and Hostâ€“Guest Interaction of Histidine-Intercalated Hydrotalciteâ€“Montmorillonite Complex. Minerals (Basel, Switzerland), 2018, 8, 198.	2.0	4

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37	Density functional theoretical studies on the ring-opening polymerization mechanism of oxetane cation series compounds. RSC Advances, 2017, 7, 49626-49632.	3.6	2
38	DFTâ€Based Simulation and Experimental Validation of the Topotactic Transformation of MgAl Layered Double Hydroxides. ChemPhysChem, 2016, 17, 2754-2766.	2.1	30
39	Density functional theory study of the mechanism of a dipeptide-catalyzed intermolecular aldol reactionâ€"the effects of steric repulsion interactions on stereoselectivity. RSC Advances, 2016, 6, 19742-19750.	3.6	2
40	Analysis and simulations on the structure of sulfanilic acid zwitterion intercalated hydrotalcite and montmorillonite. RSC Advances, 2016, 6, 83656-83662.	3.6	1
41	Ru-Cluster-Modified Ni Surface Defects toward Selective Bond Breaking between Câ€‘O and Câ€‘C. Chemistry of Materials, 2016, 28, 4751-4761.	6.7	37
42	Theoretical studies of structure and racemization mechanism of aspartate-intercalated hydrotalcite. Research on Chemical Intermediates, 2016, 42, 5835-5848.	2.7	1
43	TiO₂@Layered Double Hydroxide Coreâ€“Shell Nanospheres with Largely Enhanced Photocatalytic Activity Toward O₂ Generation. Advanced Functional Materials, 2015, 25, 2243-2249.	14.9	223
44	A density functional theory study of gold clusters supported on layered double hydroxides. Structural Chemistry, 2014, 25, 883-893.	2.0	4
45	The effect of palladium clusters (Pdn, n=2â€“8) on mechanisms of acetylene hydrogenation: A DFT study. Journal of Molecular Catalysis A, 2012, 359, 14-20.	4.8	35
46	Theoretical study of two photochemical pathways of l-tyrosine isomerization. Journal of Molecular Structure, 2012, 1015, 106-111.	3.6	9
47	Study of cisâ€“trans isomerization mechanism of 3,3â€²-azobenzene disulphonate in the lowest singlet and triplet electronic states by density functional theory. Structural Chemistry, 2010, 21, 817-825.	2.0	1
48	Supramolecular structural control and characteristics of p-hydroxybenzoate intercalated hydrotalcite. Journal of Physics and Chemistry of Solids, 2010, 71, 1290-1294.	4.0	10
49	A density functional theory study on the thermal and photochemical isomerization mechanism of 4,4â€²-azobenzene disulfonate. Journal of Photochemistry and Photobiology A: Chemistry, 2010, 211, 89-98.	3.9	3
50	Synthesis and structural characterization of mordant yellow 10-pillared magnesiumâ€“aluminum layered double hydroxides. Journal of Physics and Chemistry of Solids, 2008, 69, 1084-1087.	4.0	12
51	Quantum chemistry and molecular mechanics studies of the lamella structure of hydrotalcite with Mg/Al ratio of 3. Journal of Physics and Chemistry of Solids, 2008, 69, 1066-1069.	4.0	9
52	Theoretical study of formation mechanism of aluminosilicate in the synthesis of zeolites. Structural Chemistry, 2008, 19, 481-487.	2.0	12
53	Intercalation of <scp>l</scp>-Dopa into Layered Double Hydroxides: Enhancement of Both Chemical and Stereochemical Stabilities of a Drug through Hostâ^'Guest Interactions. Chemistry of Materials, 2008, 20, 5169-5180.	6.7	107
54	Theoretical study of two pathways of double-bond isomerization of pentene catalyzed by zeolites. Computational Materials Science, 2008, 42, 179-185.	3.0	9

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55	Theoretical study of the cracking mechanisms of linear Î±-olefins catalyzed by zeolites. Applied Surface Science, 2007, 254, 604-609.	6.1	22
56	Catalytic isomerization of 1-pentene to cis-2-pentene over zeolites: A quantum mechanical study. Materials Chemistry and Physics, 2007, 106, 394-398.	4.0	3
57	Experimental and theoretical study on the structure of acid orange 7-pillared layered double hydroxide. Materials Chemistry and Physics, 2007, 106, 422-427.	4.0	28
58	Preparation and characterization of l-cystine and l-cysteine intercalated layered double hydroxides. Journal of Materials Science, 2007, 42, 2684-2689.	3.7	34
59	Preparation and thermal decomposition studies of l-tyrosine intercalated MgAl, NiAl and ZnAl layered double hydroxides. Journal of Physics and Chemistry of Solids, 2006, 67, 1469-1476.	4.0	40
60	Theoretical studies on the butene double bond isomerization catalyzed by 5-H of 1-ethyl-3-methyl-imidazolium fluoride. Structural Chemistry, 2006, 17, 377-381.	2.0	3
61	Study on the Photochromism of Niâ€“Al Layered Double Hydroxides Containing Nitrate Anions. European Journal of Inorganic Chemistry, 2006, 2006, 2831-2838.	2.0	69
62	Study of the In Situ Postintercalative Polymerization of Metanilic Anions Intercalated in NiAl-Layered Double Hydroxides under a Nitrogen Atmosphere. European Journal of Inorganic Chemistry, 2006, 2006, 3442-3450.	2.0	22
63	A density-functional theory study on double-bond isomerization of 1-butene to cis-2-butene catalyzed by zeolites. Chemical Physics Letters, 2005, 404, 384-388.	2.6	23
64	Theoretical study on the microstructures of hydrotalcite lamellae with Mg/Al ratio of two. Materials Letters, 2005, 59, 3343-3347.	2.6	23
65	Theoretical Study on the Mechanism of the Benzaldehydes Deoxyfluorination by Sulfuryl Fluoride and Tetramethylammonium Fluoride. Journal of Physical Organic Chemistry, 0, , .	1.9	1