Hua-Qing Yang

List of Publications by Year
in descending order

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51	873	516710 16	526287 27
papers	citations	h-index	g-index

52	52	52	1032
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Production of high-grade diesel from palmitic acid over activated carbon-supported nickel phosphide catalysts. Applied Catalysis B: Environmental, 2016, 187, 375-385.	20.2	113
2	Performance of Dimethyl Sulfoxide and BrÃ¸nsted Acid Catalysts in Fructose Conversion to 5-Hydroxymethylfurfural. ACS Catalysis, 2017, 7, 2199-2212.	11.2	100
3	General low-temperature reaction pathway from precursors to monomers before nucleation of compound semiconductor nanocrystals. Nature Communications, 2016, 7, 12223.	12.8	44
4	Promotion catalytic role of ethanol on BrÃ¸nsted acid for the sequential dehydration-etherification of fructose to 5-ethoxymethylfurfural. Journal of Catalysis, 2017, 352, 586-598.	6.2	40
5	Chitosan/Sulfobutylether-Î²-Cyclodextrin Nanoparticles for Ibrutinib Delivery: A Potential Nanoformulation of Novel Kinase Inhibitor. Journal of Pharmaceutical Sciences, 2020, 109, 1136-1144.	3.3	31
6	Theoretical study of the catalytic oxidation mechanism of 5-hydroxymethylfurfural to 2,5-diformylfuran by PMo-containing Keggin heteropolyacid. Catalysis Science and Technology, 2016, 6, 3776-3787.	4.1	29
7	Adjusting the acidity of sulfonated organocatalyst for the one-pot production of 5-ethoxymethylfurfural from fructose. Catalysis Science and Technology, 2019, 9, 483-492.	4.1	28
8	Cooperative Catalytic Performance of Lewis and BrÃ¸nsted Acids from AlCl₃ Salt in Aqueous Solution toward Glucose-to-Fructose Isomerization. Journal of Physical Chemistry C, 2019, 123, 4879-4891.	3.1	28
9	Theoretical Study on the Mechanism of the Reaction of CH4+ MgO. Journal of Physical Chemistry A, 2003, 107, 2316-2323.	2.5	27
10	Theoretical study on the reaction mechanism of CH4 with CaO. Chemical Physics, 2006, 330, 343-348.	1.9	26
11	One-step synthesis of ultrabright amphiphilic carbon dots for rapid and precise tracking lipid droplets dynamics in biosystems. Biosensors and Bioelectronics, 2022, 200, 113928.	10.1	26
12	Catalytic Dehydration of Fructose into 5â€Hydroxymethylfurfural by a DMSOâ€like Polymeric Solid Organocatalyst. ChemCatChem, 2017, 9, 3218-3225.	3.7	25
13	Mechanistic Study of the Role of Primary Amines in Precursor Conversions to Semiconductor Nanocrystals at Low Temperature. Angewandte Chemie - International Edition, 2014, 53, 6898-6904.	13.8	24
14	Theoretical Insight into the Coordination of Cyclic Î²-<scp>d</scp>-Glucose to [Al(OH)(aq)]²⁺ and [Al(OH)₂(aq)]¹⁺ Ions. Journal of Physical Chemistry B, 2014, 118, 13890-13902.	2.6	23
15	Synergistic Catalytic Mechanism of Acidic Silanol and Basic Alkylamine Bifunctional Groups Over SBA-15 Zeolite toward Aldol Condensation. Journal of Physical Chemistry C, 2019, 123, 4903-4913.	3.1	20
16	Theoretical study on the reaction of methane and zinc oxide in gas phase. Computational and Theoretical Chemistry, 2006, 778, 41-48.	1.5	19
17	Activation of Câ€“H and Câ€“C bonds of ethane by gas-phase Pt atom: Potential energy surface and reaction mechanism. Computational and Theoretical Chemistry, 2012, 994, 112-120.	2.5	16
18	Activation of Propane C-H and C-C Bonds by Gas-Phase Pt Atom: A Theoretical Study. International Journal of Molecular Sciences, 2012, 13, 9278-9297.	4.1	15

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19	Catalytic mechanisms of oxygen-containing groups over vanadium active sites in an Al-MCM-41 framework for production of 2,5-diformylfuran from 5-hydroxymethylfurfural. Catalysis Science and Technology, 2020, 10, 278-290.	4.1	15
20	Theoretical Study on the Catalytic Reduction Mechanism of NO by CO on Tetrahedral Rh4 Subnanocluster. Journal of Physical Chemistry A, 2015, 119, 11548-11564.	2.5	13
21	Density Functional Theory Study on the Nucleation and Growth of Pt_n Clusters on Î³-Al₂O₃(001) Surface. ACS Omega, 2017, 2, 3250-3259.	3.5	13
22	Performance of edges on carbon for the catalytic hydroxylation of benzene to phenol. Catalysis Science and Technology, 2018, 8, 176-186.	4.1	13
23	The design and catalytic performance of molybdenum active sites on an MCM-41 framework for the aerobic oxidation of 5-hydroxymethylfurfural to 2,5-diformylfuran. Catalysis Science and Technology, 2019, 9, 811-821.	4.1	13
24	Fabrication of carboxymethyl functionalized Î²-cyclodextrin-modified graphene oxide for efficient removal of methylene blue. Arabian Journal of Chemistry, 2020, 13, 7020-7031.	4.9	13
25	Catalytic reduction of NO by CO on Rh₄⁺ clusters: a density functional theory study. Catalysis Science and Technology, 2015, 5, 3203-3215.	4.1	12
26	Catalytic Mechanisms of Zirconium-Containing Active Sites over the SBA-15 Zeolite Framework for Xylose Conversion to Methyl Lactate. Journal of Physical Chemistry C, 2020, 124, 13102-13112.	3.1	11
27	Mechanistic study of cellobiose conversion to 5-hydroxymethylfurfural catalyzed by a BrÃ¸nsted acid with counteranions in an aqueous solution. Physical Chemistry Chemical Physics, 2020, 22, 9349-9361.	2.8	11
28	Reaction mechanism on the activation of ethane Câ€“H and Câ€“C bonds by a diplatinum cluster. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	10
29	Theoretical study on the reaction mechanism of NO and CO catalyzed by Rh atom. Structural Chemistry, 2013, 24, 13-23.	2.0	9
30	Activation of propane Câ€“H and Câ€“C bonds by a diplatinum cluster: potential energy surfaces and reaction mechanisms. Structural Chemistry, 2014, 25, 471-481.	2.0	9
31	Theoretical study on the gasâ€phase reaction mechanism between rhodium monoxide and methane for methanol production. Journal of Computational Chemistry, 2010, 31, 938-953.	3.3	8
32	Theoretical investigation on copper hydrides catalyzed hydrosilylation reaction of 3-methylcyclohex-2-enone: mechanism and ligands' effect. Catalysis Science and Technology, 2012, 2, 564-569.	4.1	8
33	Molecular mechanism comparison of decarbonylation with deoxygenation and hydrogenation of 5-hydroxymethylfurfural catalyzed by palladium acetate. Physical Chemistry Chemical Physics, 2019, 21, 3795-3804.	2.8	8
34	Catalytic mechanism for the isomerization of glucose into fructose over an aluminium-MCM-41 framework. Catalysis Science and Technology, 2021, 11, 1537-1543.	4.1	8
35	Insights into the Mechanistic Role of Diphenylphosphine Selenide, Diphenylphosphine, and Primary Amines in the Formation of CdSe Monomers. Journal of Physical Chemistry A, 2016, 120, 918-931.	2.5	7
36	Theoretical Study on Heteroâ€Dielsâ€“Alder Reaction of Butadiene with Benzaldehyde Catalyzed by Chiral In^{III} Complexes. European Journal of Organic Chemistry, 2010, 2010, 3867-3875.	2.4	6

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37	Theoretical study on the gas-phase reaction mechanism between rhodium monoxide cation and methane. Structural Chemistry, 2011, 22, 983-997.	2.0	6
38	Theoretical study on the gasâ€phase reaction mechanism between palladium monoxide and methane. Journal of Computational Chemistry, 2011, 32, 3440-3455.	3.3	6
39	A DFT STUDY ON THE REACTION MECHANISM OF SrO + CH4. Journal of Theoretical and Computational Chemistry, 2008, 07, 189-203.	1.8	5
40	Theoretical study on the gasâ€phase reaction mechanism between nickel monoxide and methane for syngas production. Journal of Computational Chemistry, 2009, 30, 847-863.	3.3	5
41	Theoretical Insights into the Cooperative Catalytic Mechanism of a PW-Containing Keggin Heteropolyacid Anion and Ethanol toward Conversion of Fructose into 5-Ethoxymethylfurfural in Ethanol Solution. ACS Sustainable Chemistry and Engineering, 2021, 9, 14789-14799.	6.7	5
42	Methane dehydrogenation on monomeric Rh center located on (100) Î³-alumina â€" A theoretical study. Surface Science, 2012, 606, 1899-1905.	1.9	4
43	Theoretical insight into the Câ€"H and Câ€"C scission mechanism of ethane on a tetrahedral Pt₄subnanocluster. RSC Advances, 2015, 5, 40978-40988.	3.6	4
44	Mechanism of Preferential Hydrogenation of Hydroxymethyl Group to Aldehyde Group in 5â€Hydroxymethylfurfural over W₂Câ€Based Catalyst. ChemSusChem, 2022, 15, e202200174.	6.8	4
45	Cooperative interaction of sodium and chlorine ions with Î²-cellobiose in aqueous solution from quantum mechanics and molecular dynamics. Cellulose, 2020, 27, 6793-6809.	4.9	3
46	Theoretical insight into the deoxygenation molecular mechanism of butyric acid catalyzed by a Ni₁₂P₆ cluster. Catalysis Science and Technology, 2021, 11, 6425-6437.	4.1	2
47	Catalytic performance of Pt3Ni cluster toward ethane activation. Chemical Physics, 2021, 548, 111204.	1.9	2
48	THEORETICAL STUDY ON METHANE HYDROXYLATION BY MIMIC METHANE MONOOXYGENASE WITH bis(Î¼-OXO)DIMANGANESE CORE. Journal of Theoretical and Computational Chemistry, 2010, 09, 233-247.	1.8	1
49	Regular patterns of the effects of hydrogen-containing additives on the formation of CdSe monomer. Physical Chemistry Chemical Physics, 2018, 20, 20863-20873.	2.8	1
50	Theoretical study on molecular mechanism of aerobic oxidation of 5-hydroxymethylfurfural to 2,5-diformyfuran catalyzed by VO2+ with counterpart anion in N,N-dimethylacetamide solution. RSC Advances, 2021, 11, 39888-39895.	3.6	1
51	Mechanism Insight into Catalytic Performance of Ni12P5 over Ni2P toward the Catalytic Deoxygenation of Butyric Acid. Catalysts, 2022, 12, 569.	3.5	1