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	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
2	Mechanism of Preferential Hydrogenation of Hydroxymethyl Group to Aldehyde Group in 5â€Hydroxymethylfurfural over W₂Câ€Based Catalyst. ChemSusChem, 2022, 15, e202200174.	6.8	4
3	Mechanism Insight into Catalytic Performance of Ni12P5 over Ni2P toward the Catalytic Deoxygenation of Butyric Acid. Catalysts, 2022, 12, 569.	3.5	1
4	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
5	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
6	Catalytic performance of Pt3Ni cluster toward ethane activation. Chemical Physics, 2021, 548, 111204.	1.9	2
7	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
8	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
9	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
10	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
11	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
12	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
13	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
14	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
15	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
16	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
17	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
18	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

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19	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
20	Performance of edges on carbon for the catalytic hydroxylation of benzene to phenol. Catalysis Science and Technology, 2018, 8, 176-186.	4.1	13
21	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
22	Catalytic Dehydration of Fructose into 5â€Hydroxymethylfurfural by a DMSOâ€like Polymeric Solid Organocatalyst. ChemCatChem, 2017, 9, 3218-3225.	3.7	25
23	Performance of Dimethyl Sulfoxide and BrÃ¸nsted Acid Catalysts in Fructose Conversion to 5-Hydroxymethylfurfural. ACS Catalysis, 2017, 7, 2199-2212.	11.2	100
24	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
25	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
26	General low-temperature reaction pathway from precursors to monomers before nucleation of compound semiconductor nanocrystals. Nature Communications, 2016, 7, 12223.	12.8	44
27	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
28	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
29	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
30	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
31	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
32	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
33	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
34	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
35	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
36	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

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37	Theoretical study on the reaction mechanism of NO and CO catalyzed by Rh atom. Structural Chemistry, 2013, 24, 13-23.	2.0	9
38	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
39	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
40	Methane dehydrogenation on monomeric Rh center located on (100) Î³-alumina â€" A theoretical study. Surface Science, 2012, 606, 1899-1905.	1.9	4
41	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
42	Theoretical study on the gas-phase reaction mechanism between rhodium monoxide cation and methane. Structural Chemistry, 2011, 22, 983-997.	2.0	6
43	Theoretical study on the gasâ€phase reaction mechanism between palladium monoxide and methane. Journal of Computational Chemistry, 2011, 32, 3440-3455.	3.3	6
44	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
45	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
46	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
47	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
48	A DFT STUDY ON THE REACTION MECHANISM OF SrO + CH4. Journal of Theoretical and Computational Chemistry, 2008, 07, 189-203.	1.8	5
49	Theoretical study on the reaction of methane and zinc oxide in gas phase. Computational and Theoretical Chemistry, 2006, 778, 41-48.	1.5	19
50	Theoretical study on the reaction mechanism of CH4 with CaO. Chemical Physics, 2006, 330, 343-348.	1.9	26
51	Theoretical Study on the Mechanism of the Reaction of CH4+ MgO. Journal of Physical Chemistry A, 2003, 107, 2316-2323.	2.5	27