

Hua-Jun S Fan

List of Publications by Year in descending order

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36
papers

1,243
citations

567281

15
h-index

434195

31
g-index

39
all docs

39
docs citations

39
times ranked

1550
citing authors

#	ARTICLE	IF	CITATIONS
1	A Capable Bridging Ligand for Fe-Only Hydrogenase: Density Functional Calculations of a Low-Energy Route for Heterolytic Cleavage and Formation of Dihydrogen. <i>Journal of the American Chemical Society</i> , 2001, 123, 3828-3829.	13.7	334
2	Thermally Stable Homogeneous Catalysts for Alkane Dehydrogenation S.O. thanks the German Academic Exchange Service (DAAD) for financing a research stay with W.C.K. in the USA. This work was supported by the National Science Foundation (CHE 9800184 to M.B.H.), by the University of California Energy Institute and University of California Santa Barbara (to W.C.K.), and by the German Research Association (DFG, to M.W.H). We thank Dr. R. Mynott and Mrs. C. Wirtz, MPI für Kohlenforschung, for NMR spectroscopic in. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 3596.	13.8	175
3	Molecular Control of the Nanoscale: Effect of Phosphine-Chalcogenide Reactivity on CdS-CdSe Nanocrystal Composition and Morphology. <i>ACS Nano</i> , 2012, 6, 5348-5359.	14.6	101
4	Density functional study of the catalytic cycle of nickel-iron [NiFe] hydrogenases and the involvement of high-spin nickel(II). <i>Journal of Biological Inorganic Chemistry</i> , 2006, 11, 286-306.	2.6	83
5	IR spectroelectrochemical study of the binding of carbon monoxide to the active site of <i>Desulfovibrio fructosovorans</i> Ni-Fe hydrogenase. <i>Journal of Biological Inorganic Chemistry</i> , 2002, 7, 318-326.	2.6	78
6	Synthesis and characterization of Fe ₃ O ₄ /ZnO-GO nanocomposites with improved photocatalytic degradation methyl orange under visible light irradiation. <i>Journal of Alloys and Compounds</i> , 2018, 737, 197-206.	5.5	78
7	Phase-Programmed Nanofabrication: Effect of Organophosphite Precursor Reactivity on the Evolution of Nickel and Nickel Phosphide Nanocrystals. <i>Chemistry of Materials</i> , 2015, 27, 8021-8031.	6.7	44
8	High-Spin Ni(II), a Surprisingly Good Structural Model for [NiFe] Hydrogenase. <i>Journal of the American Chemical Society</i> , 2002, 124, 394-395.	13.7	43
9	Equilibrium Solubility, Model Correlation, and Solvent Effect of Indole-3-acetic Acid in Twelve Pure Solvents. <i>Journal of Chemical & Engineering Data</i> , 2019, 64, 1802-1808.	1.9	37
10	Recent theoretical predictions of the active site for the observed forms in the catalytic cycle of Ni-Fe hydrogenase. <i>Journal of Biological Inorganic Chemistry</i> , 2001, 6, 467-473.	2.6	32
11	Carbon quantum dots interfacial modified graphene/silicon Schottky barrier solar cell. <i>Journal of Alloys and Compounds</i> , 2020, 835, 155268.	5.5	21
12	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms. 19. Substitution Reaction in Cyclopentadienyl Metal Dicarboxyls. <i>Organometallics</i> , 2001, 20, 5724-5730.	2.3	20
13	Ligand-mediated metal-metal interactions and localized versus delocalized mixed-valence cation states of biferrocene and bis(1/4-fulvalenediyl)diiron characterized in the gas phase by valence photoelectron spectroscopy. <i>Journal of Organometallic Chemistry</i> , 2003, 666, 75-85.	1.8	19
14	Assessing Phosphine-Chalcogen Bond Energetics from Calculations. <i>Organometallics</i> , 2015, 34, 4023-4031.	2.3	19
15	High-performance Si/nano-Cu/CNTs/C anode derived from photovoltaic silicon waste: A potential photovoltaic-energy storage strategy. <i>Materials Today Energy</i> , 2021, 20, 100671.	4.7	17
16	Electronic Structure of Early Transition-Metal Carbonyls: Gas-Phase Photoelectron Spectroscopy of (1/5-C ₅ H ₅)M(CO) ₄ (M = V, Nb, Ta). <i>Organometallics</i> , 2000, 19, 2012-2021.	2.3	15
17	Density functional studies of catalytic alkane dehydrogenation by an iridium pincer complex with and without a hydrogen acceptor. <i>Journal of Molecular Catalysis A</i> , 2002, 189, 111-118.	4.8	15
18	Enhance the interaction between ammonium polyphosphate and epoxy resin matrix through hydrophobic modification with cationic latex. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2021, 610, 125917.	4.7	15

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19	Calcium-cross linked polysaccharide microcapsules for controlled release and antimicrobial applications. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2020, 600, 125025.	4.7	13
20	The improved hydrodechlorination catalytic reactions by concerted efforts of ionic liquid and activated carbon support. <i>New Journal of Chemistry</i> , 2019, 43, 6659-6665.	2.8	12
21	Synthesis, crystal structure and investigation of mononuclear copper(II) and zinc(II) complexes of a new carboxylate rich tripodal ligand and their interaction with carbohydrates in alkaline aqueous solution. <i>Journal of Inorganic Biochemistry</i> , 2015, 149, 25-38.	3.5	11
22	Intermetallic Nanocatalysts from Heterobimetallic Group 10â€“14 Pyridine-2-thiolate Precursors. <i>Organometallics</i> , 2020, 39, 1092-1104.	2.3	11
23	A Newly Designed Carbohydrate-Derived Alkylamine Promotes Ullmann Type Câ€“N Coupling Catalyzed by Copper in Water. <i>Synlett</i> , 2019, 30, 193-198.	1.8	10
24	DENSITY FUNCTIONAL STUDIES OF IRIDIUM CATALYZED ALKANE DEHYDROGENATION. <i>Advances in Inorganic Chemistry</i> , 2003, , 321-349.	1.0	8
25	Teaching Chemistry with Computers. <i>International Journal of Information and Education Technology</i> , 2015, 5, 184-188.	1.2	7
26	Origin of the Regioselectivity in the Aldol Condensation between Hydroxymethylfurfural and Levulinic Acid: A DFT Investigation. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1985-1992.	2.5	6
27	Solubility and Thermodynamic Model Correlation of Zonisamide in Different Pure Solvents from $T = 273.15$ to 313.15 K. <i>Journal of Chemical & Engineering Data</i> , 2020, 65, 3637-3644.	1.9	6
28	Research on the 2-Chloro-4-amino-6,7-dimethoxyquinazoline Solubility in 12 Monosolvents at Various Temperatures: Experimental Measurement and Thermodynamic Correlation. <i>Journal of Chemical & Engineering Data</i> , 2021, 66, 170-177.	1.9	6
29	Heteroleptic dmit nickel complexes with bis(diphenylphosphanyl)amine ligands as robust molecular electrocatalysts for hydrogen evolution. <i>Applied Organometallic Chemistry</i> , 2021, 35, .	3.5	3
30	A DFT study on the mechanism of Wolff Rearrangement in a five-membered Iridacycle. <i>Procedia Computer Science</i> , 2010, 1, 2659-2667.	2.0	2
31	Polyionic Liquids (PIL) Promoted Ce Doped ZnO for the Photocatalytic Degradation of Rhodamine B (RhB). <i>ChemistrySelect</i> , 2019, 4, 10748-10755.	1.5	2
32	Density Functional Studies of Catalytic Alkane Dehydrogenation by an Iridium Pincer Complex with and without a Hydrogen Acceptor. <i>ChemInform</i> , 2003, 34, no.	0.0	0
33	Density Functional Studies of Iridium-Catalyzed Alkane Dehydrogenation. <i>ChemInform</i> , 2004, 35, no.	0.0	0
34	The Impact of p-orbital on Optimization of $\text{ReH}_7(\text{PMe}_3)_2$ Compound. <i>Procedia Computer Science</i> , 2014, 29, 1376-1383.	2.0	0
35	4,6-Di-O-Benzylidene group-directed preparation of 2-deoxy-2-azido- α -D-galactopyranosides promoted by 3-O-TBDPS. <i>Carbohydrate Research</i> , 2021, 500, 108237.	2.3	0
36	Synthesis and Modeling of Transition Metal Complexes Using Histidine as the Ligand.. <i>Frontiers in Chemistry</i> , 0, 6, .	3.6	0