

Zhi-Jian Zhao

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

136 papers	13,161 citations	60 h-index	114 g-index
148 ext. papers	16,229 ext. citations	14.6 avg, IF	7.21 L-index

#	Paper	IF	Citations
136	Moderate Surface Segregation Promotes Selective Ethanol Production in CO ₂ Hydrogenation Reaction over CoCu Catalysts. <i>Angewandte Chemie</i> , 2022 , 134, e202109027	3.6	2
135	Dynamics of Heterogeneous Catalytic Processes at Operando Conditions.. <i>Jacs Au</i> , 2021 , 1, 2100-2120		4
134	Black phosphorus-hosted single-atom catalyst for electrocatalytic nitrogen reduction. <i>Science China Materials</i> , 2021 , 64, 1173-1181	7.1	8
133	On the Role of Sn Segregation of Pt-Sn Catalysts for Propane Dehydrogenation. <i>ACS Catalysis</i> , 2021 , 11, 4401-4410	13.1	16
132	Tandem catalysis at nanoscale. <i>Science</i> , 2021 , 371, 1203-1204	33.3	2
131	Artificial Leaves for Solar Fuels. <i>Chinese Journal of Chemistry</i> , 2021 , 39, 1450-1458	4.9	2
130	Controllable Cu ⁰ -Cu ⁺ Sites for Electrocatalytic Reduction of Carbon Dioxide. <i>Angewandte Chemie</i> , 2021 , 133, 15472-15475	3.6	12
129	Origin of Performances of Pt/Cu Single-Atom Alloy Catalysts for Propane Dehydrogenation. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 18708-18716	3.8	8
128	Controllable Distribution of Oxygen Vacancies in Grain Boundaries of p-Si/TiO Heterojunction Photocathodes for Solar Water Splitting. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 4034-4037	16.4	12
127	Controllable Distribution of Oxygen Vacancies in Grain Boundaries of p-Si/TiO ₂ Heterojunction Photocathodes for Solar Water Splitting. <i>Angewandte Chemie</i> , 2021 , 133, 4080-4083	3.6	4
126	The nature of active sites for carbon dioxide electroreduction over oxide-derived copper catalysts. <i>Nature Communications</i> , 2021 , 12, 395	17.4	46
125	Shale gas revolution: Catalytic conversion of C ₁ -C ₃ light alkanes to value-added chemicals. <i>Chem</i> , 2021 , 7, 1755-1801	16.2	11
124	Effect of bicarbonate on CO ₂ electroreduction over cathode catalysts. <i>Fundamental Research</i> , 2021 , 1, 432-438		4
123	Efficient CO electroreduction on facet-selective copper films with high conversion rate. <i>Nature Communications</i> , 2021 , 12, 5745	17.4	19
122	Propane dehydrogenation: catalyst development, new chemistry, and emerging technologies. <i>Chemical Society Reviews</i> , 2021 , 50, 3315-3354	58.5	95
121	Strong Electronic Oxide-Support Interaction over InO/ZrO for Highly Selective CO Hydrogenation to Methanol. <i>Journal of the American Chemical Society</i> , 2020 , 142, 19523-19531	16.4	55
120	FeO Octahedral Distortion Activates Lattice Oxygen in Perovskite Ferrite for Methane Partial Oxidation Coupled with CO Splitting. <i>Journal of the American Chemical Society</i> , 2020 , 142, 11540-11549	16.4	65

119	Facilitating the reduction of V-O bonds on VO /ZrO catalysts for non-oxidative propane dehydrogenation. <i>Chemical Science</i> , 2020 , 11, 3845-3851	9.4	34
118	Selective Electroreduction of Carbon Dioxide over SnO -Nanodot Catalysts. <i>ChemSusChem</i> , 2020 , 13, 6353-6359	8.3	3
117	Grain-Boundary-Rich Copper for Efficient Solar-Driven Electrochemical CO Reduction to Ethylene and Ethanol. <i>Journal of the American Chemical Society</i> , 2020 , 142, 6878-6883	16.4	121
116	Tuning Oxygen Vacancies of Oxides to Promote Electrocatalytic Reduction of Carbon Dioxide. <i>ACS Energy Letters</i> , 2020 , 5, 552-558	20.1	19
115	Alternative Strategies Toward Sustainable Ammonia Synthesis. <i>Transactions of Tianjin University</i> , 2020 , 26, 67-91	2.9	18
114	Chemical looping steam reforming of methane over Ce-doped perovskites. <i>Chemical Engineering Science</i> , 2020 , 223, 115707	4.4	14
113	Concentrating and activating carbon dioxide over AuCu aerogel grain boundaries. <i>Journal of Chemical Physics</i> , 2020 , 152, 204703	3.9	6
112	Enriched Surface Oxygen Vacancies of Photoanodes by Photoetching with Enhanced Charge Separation. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 2044-2048	16.4	83
111	Exploring the initial oxidation of Pt, Pt3Ni, Pt3Au (111) surfaces: a genetic algorithm based global optimization with density functional theory. <i>Green Chemical Engineering</i> , 2020 , 1, 56-62	3	6
110	Golden touch of the nanoparticles. <i>Nature Nanotechnology</i> , 2020 , 15, 1-2	28.7	8
109	Defect-mediated reactivity of Pt/TiO2 catalysts: the different role of titanium and oxygen vacancies. <i>Science China Chemistry</i> , 2020 , 63, 1323-1330	7.9	10
108	Theoretical insights into single-atom catalysts. <i>Chemical Society Reviews</i> , 2020 , 49, 8156-8178	58.5	89
107	Coverage-Dependent Behaviors of Vanadium Oxides for Chemical Looping Oxidative Dehydrogenation. <i>Angewandte Chemie</i> , 2020 , 132, 22256-22263	3.6	2
106	Nanostructured Catalysts toward Efficient Propane Dehydrogenation. <i>Accounts of Materials Research</i> , 2020 , 1, 30-40	7.5	22
105	Operando characterization techniques for electrocatalysis. <i>Energy and Environmental Science</i> , 2020 , 13, 3748-3779	35.4	83
104	Pt/Pd Single-Atom Alloys as Highly Active Electrochemical Catalysts and the Origin of Enhanced Activity. <i>ACS Catalysis</i> , 2019 , 9, 9350-9358	13.1	61
103	Achieving efficient and robust catalytic reforming on dual-sites of Cu species. <i>Chemical Science</i> , 2019 , 10, 2578-2584	9.4	24
102	Crucial Role of Surface Hydroxyls on the Activity and Stability in Electrochemical CO Reduction. <i>Journal of the American Chemical Society</i> , 2019 , 141, 2911-2915	16.4	115

101	Gold nanorods-based hybrids with tailored structures for photoredox catalysis: fundamental science, materials design and applications. <i>Nano Today</i> , 2019 , 27, 48-72	17.9	65
100	Theory assisted design of N-doped tin oxides for enhanced electrochemical CO ₂ activation and reduction. <i>Science China Chemistry</i> , 2019 , 62, 1030-1036	7.9	17
99	Structure-Performance Relationships for Propane Dehydrogenation over Aluminum Supported Vanadium Oxide. <i>ACS Catalysis</i> , 2019 , 9, 5816-5827	13.1	45
98	Adsorption Preference Determines Segregation Direction: A Shortcut to More Realistic Surface Models of Alloy Catalysts. <i>ACS Catalysis</i> , 2019 , 9, 5011-5018	13.1	19
97	Fabrication of bilayer Pd-Pt nanocages with sub-nanometer thin shells for enhanced hydrogen evolution reaction. <i>Nano Research</i> , 2019 , 12, 2268-2274	10	23
96	Ultrathin Pd-Au Shells with Controllable Alloying Degree on Pd Nanocubes toward Carbon Dioxide Reduction. <i>Journal of the American Chemical Society</i> , 2019 , 141, 4791-4794	16.4	85
95	Abundant Ce Ions in Au-CeO Nanosheets to Enhance CO Electroreduction Performance. <i>Small</i> , 2019 , 15, e1900289	11	25
94	Symmetry-Breaking Synthesis of Multicomponent Nanoparticles. <i>Accounts of Chemical Research</i> , 2019 , 52, 1125-1133	24.3	40
93	Hydroxyl-mediated ethanol selectivity of CO hydrogenation. <i>Chemical Science</i> , 2019 , 10, 3161-3167	9.4	65
92	Single-Atom Mn-N Site-Catalyzed Peroxone Reaction for the Efficient Production of Hydroxyl Radicals in an Acidic Solution. <i>Journal of the American Chemical Society</i> , 2019 , 141, 12005-12010	16.4	94
91	Modulating Lattice Oxygen in Dual-Functional Mo-V-O Mixed Oxides for Chemical Looping Oxidative Dehydrogenation. <i>Journal of the American Chemical Society</i> , 2019 , 141, 18653-18657	16.4	65
90	Active sites in CO ₂ hydrogenation over confined VO _x -Rh catalysts. <i>Science China Chemistry</i> , 2019 , 62, 1710-1719	7.9	19
89	Theory-guided design of catalytic materials using scaling relationships and reactivity descriptors. <i>Nature Reviews Materials</i> , 2019 , 4, 792-804	73.3	164
88	Insights into interface engineering in steam reforming reactions for hydrogen production. <i>Energy and Environmental Science</i> , 2019 , 12, 3473-3495	35.4	47
87	Modulating the surface defects of titanium oxides and consequent reactivity of Pt catalysts. <i>Chemical Science</i> , 2019 , 10, 10531-10536	9.4	6
86	Facet-evolution growth of Mn ₃ O ₄ @Co _x Mn _{3-x} O ₄ electrocatalysts on Ni foam towards efficient oxygen evolution reaction. <i>Journal of Catalysis</i> , 2019 , 369, 105-110	7.3	22
85	A welding phenomenon of dissimilar nanoparticles in dispersion. <i>Nature Communications</i> , 2019 , 10, 219	17.4	11
84	Competition of C-C bond formation and C-H bond formation For acetylene hydrogenation on transition metals: A density functional theory study. <i>AIChE Journal</i> , 2019 , 65, 1059-1066	3.6	29

83	Facet design promotes electroreduction of carbon dioxide to carbon monoxide on palladium nanocrystals. <i>Chemical Engineering Science</i> , 2019 , 194, 29-35	4.4	26
82	Promoted Fixation of Molecular Nitrogen with Surface Oxygen Vacancies on Plasmon-Enhanced TiO Photoelectrodes. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 5278-5282	16.4	271
81	Promoted Fixation of Molecular Nitrogen with Surface Oxygen Vacancies on Plasmon-Enhanced TiO ₂ Photoelectrodes. <i>Angewandte Chemie</i> , 2018 , 130, 5376-5380	3.6	37
80	On the role of Ce in CO adsorption and activation over lanthanum species. <i>Chemical Science</i> , 2018 , 9, 3426-3437	9.4	29
79	Coverage Effect on the Activity of the Acetylene Semihydrogenation over Pd ₈ N Catalysts: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 6005-6013	3.8	17
78	Hydroxyl-Mediated Non-oxidative Propane Dehydrogenation over VO _x /Al ₂ O ₃ Catalysts with Improved Stability. <i>Angewandte Chemie</i> , 2018 , 130, 6907-6911	3.6	11
77	The Functionality of Surface Hydroxy Groups on the Selectivity and Activity of Carbon Dioxide Reduction over Cuprous Oxide in Aqueous Solutions. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 7724-7728	16.4	59
76	R&Ktitelbild: Promoted Fixation of Molecular Nitrogen with Surface Oxygen Vacancies on Plasmon-Enhanced TiO ₂ Photoelectrodes (Angew. Chem. 19/2018). <i>Angewandte Chemie</i> , 2018 , 130, 5656-5656	3.6	31
75	CO ₂ Electroreduction: Morphological and Compositional Design of Pd ₂ Cu Bimetallic Nanocatalysts with Controllable Product Selectivity toward CO ₂ Electroreduction (Small 7/2018). <i>Small</i> , 2018 , 14, 1870031	11.1	1
74	Synergism of Geometric Construction and Electronic Regulation: 3D Se-(NiCo)S ₂ /(OH) Nanosheets for Highly Efficient Overall Water Splitting. <i>Advanced Materials</i> , 2018 , 30, e1705538	24	193
73	Morphological and Compositional Design of Pd-Cu Bimetallic Nanocatalysts with Controllable Product Selectivity toward CO Electroreduction. <i>Small</i> , 2018 , 14, 1703314	11	65
72	The Nature of Loading-Dependent Reaction Barriers over Mixed RuO ₂ /TiO ₂ Catalysts. <i>ACS Catalysis</i> , 2018 , 8, 5526-5532	13.1	20
71	Identification of Pt-based catalysts for propane dehydrogenation a probability analysis. <i>Chemical Science</i> , 2018 , 9, 3925-3931	9.4	67
70	Hydroxyl-Mediated Non-oxidative Propane Dehydrogenation over VO _x /Al ₂ O ₃ Catalysts with Improved Stability. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 6791-6795	16.4	97
69	Selectivity of Synthesis Gas Conversion to C ₂ + Oxygenates on fcc(111) Transition-Metal Surfaces. <i>ACS Catalysis</i> , 2018 , 8, 3447-3453	13.1	48
68	Cation-exchanged zeolites for the selective oxidation of methane to methanol. <i>Catalysis Science and Technology</i> , 2018 , 8, 114-123	5.5	110
67	Selectivity Modulation of Encapsulated Palladium Nanoparticles by Zeolite Microenvironment for Biomass Catalytic Upgrading. <i>ACS Catalysis</i> , 2018 , 8, 8578-8589	13.1	67
66	Formation of Enriched Vacancies for Enhanced CO ₂ Electrocatalytic Reduction over AuCu Alloys. <i>ACS Energy Letters</i> , 2018 , 3, 2144-2149	20.1	64

65	Subsurface catalysis-mediated selectivity of dehydrogenation reaction. <i>Science Advances</i> , 2018 , 4, eaar5418	54.8	57
64	Water Splitting: Synergism of Geometric Construction and Electronic Regulation: 3D Se-(NiCo)S _x /(OH) _x Nanosheets for Highly Efficient Overall Water Splitting (Adv. Mater. 12/2018). <i>Advanced Materials</i> , 2018 , 30, 1870085	24	25
63	Tuning Cu/Cu ₂ O Interfaces for the Reduction of Carbon Dioxide to Methanol in Aqueous Solutions. <i>Angewandte Chemie</i> , 2018 , 130, 15641-15645	3.6	23
62	Titelbild: Tuning Cu/Cu ₂ O Interfaces for the Reduction of Carbon Dioxide to Methanol in Aqueous Solutions (Angew. Chem. 47/2018). <i>Angewandte Chemie</i> , 2018 , 130, 15507-15507	3.6	1
61	Selective atomic layer deposition of RuO _x catalysts on shape-controlled Pd nanocrystals with significantly enhanced hydrogen evolution activity. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 24397-24406	12	22
60	Breaking the scaling relationship via thermally stable Pt/Cu single atom alloys for catalytic dehydrogenation. <i>Nature Communications</i> , 2018 , 9, 4454	17.4	250
59	Tuning Cu/Cu ₂ O Interfaces for the Reduction of Carbon Dioxide to Methanol in Aqueous Solutions. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 15415-15419	16.4	118
58	Metal oxide redox chemistry for chemical looping processes. <i>Nature Reviews Chemistry</i> , 2018 , 2, 349-364	34.6	188
57	The Functionality of Surface Hydroxy Groups on the Selectivity and Activity of Carbon Dioxide Reduction over Cuprous Oxide in Aqueous Solutions. <i>Angewandte Chemie</i> , 2018 , 130, 7850-7854	3.6	18
56	Nano-designed semiconductors for electro- and photoelectro-catalytic conversion of carbon dioxide. <i>Chemical Society Reviews</i> , 2018 , 47, 5423-5443	58.5	119
55	Tunable syngas production from photocatalytic CO reduction with mitigated charge recombination driven by spatially separated cocatalysts. <i>Chemical Science</i> , 2018 , 9, 5334-5340	9.4	65
54	Low-Coordinated Edge Sites on Ultrathin Palladium Nanosheets Boost Carbon Dioxide Electroreduction Performance. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 11544-11548	16.4	90
53	Temperature-induced deactivation mechanism of ZnFe ₂ O ₄ for oxidative dehydrogenation of 1-butene. <i>Reaction Chemistry and Engineering</i> , 2017 , 2, 215-225	4.9	5
52	Nanostructured Materials for Heterogeneous Electrocatalytic CO Reduction and their Related Reaction Mechanisms. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 11326-11353	16.4	588
51	Nanostrukturierte Materialien für die elektrokatalytische CO ₂ -Reduktion und ihre Reaktionsmechanismen. <i>Angewandte Chemie</i> , 2017 , 129, 11482-11511	3.6	86
50	Structural motifs of water on metal oxide surfaces. <i>Chemical Society Reviews</i> , 2017 , 46, 1785-1806	58.5	127
49	Enhanced Lattice Oxygen Reactivity over Ni-Modified WO ₃ -Based Redox Catalysts for Chemical Looping Partial Oxidation of Methane. <i>ACS Catalysis</i> , 2017 , 7, 3548-3559	13.1	94
48	Facile synthesis of Pd@Pt octahedra supported on carbon for electrocatalytic applications. <i>AIChE Journal</i> , 2017 , 63, 2528-2534	3.6	12

47	Fast Prediction of CO Binding Energy via the Local Structure Effect on PtCu Alloy Surfaces. <i>Langmuir</i> , 2017 , 33, 8700-8706	4	20
46	Uncertainties in Theoretical Description of Well-Defined Heterogeneous Catalysts. <i>Studies in Surface Science and Catalysis</i> , 2017 , 177, 541-565	1.8	1
45	Importance of metal-oxide interfaces in heterogeneous catalysis: A combined DFT, microkinetic, and experimental study of water-gas shift on Au/MgO. <i>Journal of Catalysis</i> , 2017 , 345, 157-169	7.3	86
44	Structure and catalytic consequence of Mg-modified VO _x /Al ₂ O ₃ catalysts for propane dehydrogenation. <i>AIChE Journal</i> , 2017 , 63, 4911-4919	3.6	33
43	Identification of surface species by vibrational normal mode analysis. A DFT study. <i>Surface Science</i> , 2017 , 664, 233-240	1.8	1
42	Dry reforming of methane over Ni/La ₂ O ₃ nanorod catalysts with stabilized Ni nanoparticles. <i>Applied Catalysis B: Environmental</i> , 2017 , 202, 683-694	21.8	280
41	An experimental and theoretical study of glycerol oxidation to 1,3-dihydroxyacetone over bimetallic Pt-Bi catalysts. <i>AIChE Journal</i> , 2017 , 63, 705-715	3.6	45
40	Edge Sites with Unsaturated Coordination on Core-Shell Mn O @Mn Co O Nanostructures for Electrocatalytic Water Oxidation. <i>Advanced Materials</i> , 2017 , 29, 1701820	24	97
39	Structural evolution of concave trimetallic nanocubes with tunable ultra-thin shells for oxygen reduction reaction. <i>Nanoscale</i> , 2016 , 8, 16640-16649	7.7	31
38	Catalytic Reforming of Oxygenates: State of the Art and Future Prospects. <i>Chemical Reviews</i> , 2016 , 116, 11529-11653	68.1	201
37	Monocopper Active Site for Partial Methane Oxidation in Cu-Exchanged 8MR Zeolites. <i>ACS Catalysis</i> , 2016 , 6, 6531-6536	13.1	136
36	Thin Heterojunctions and Spatially Separated Cocatalysts To Simultaneously Reduce Bulk and Surface Recombination in Photocatalysts. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 13734-13738	16.4	124
35	Collapsed polymer-directed synthesis of multicomponent coaxial-like nanostructures. <i>Nature Communications</i> , 2016 , 7, 12147	17.4	29
34	Nature of the Active Sites of VO _x /Al ₂ O ₃ Catalysts for Propane Dehydrogenation. <i>ACS Catalysis</i> , 2016 , 6, 5207-5214	13.1	129
33	Effects of Ga doping on Pt/CeO ₂ -Al ₂ O ₃ catalysts for propane dehydrogenation. <i>AIChE Journal</i> , 2016 , 62, 4365-4376	3.6	61
32	Stable Aqueous Photoelectrochemical CO ₂ Reduction by a Cu ₂ O Dark Cathode with Improved Selectivity for Carbonaceous Products. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 8840-5	16.4	135
31	CO ₂ photo-reduction: insights into CO ₂ activation and reaction on surfaces of photocatalysts. <i>Energy and Environmental Science</i> , 2016 , 9, 2177-2196	35.4	1038
30	Direct Water Decomposition on Transition Metal Surfaces: Structural Dependence and Catalytic Screening. <i>Catalysis Letters</i> , 2016 , 146, 718-724	2.8	11

29	Platinum-Modified ZnO/Al ₂ O ₃ for Propane Dehydrogenation: Minimized Platinum Usage and Improved Catalytic Stability. <i>ACS Catalysis</i> , 2016 , 6, 2158-2162	13.1	113
28	Shape-controlled synthesis of Au-Pd bimetallic nanocrystals for catalytic applications. <i>Chemical Society Reviews</i> , 2016 , 45, 3916-34	58.5	193
27	Theoretical Insights into the Selective Oxidation of Methane to Methanol in Copper-Exchanged Mordenite. <i>ACS Catalysis</i> , 2016 , 6, 3760-3766	13.1	110
26	Heterogeneous Molecular Systems for Photocatalytic CO Reduction with Water Oxidation. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 14924-14950	16.4	263
25	Towards First Principles-Based Prediction of Highly Accurate Electrochemical Pourbaix Diagrams. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 18177-18187	3.8	63
24	Identification of surface intermediates during ethylidyne formation on Pt(111) by calculation of infrared intensities and deuterium isotope shifts. <i>Surface Science</i> , 2015 , 640, 112-118	1.8	15
23	Effect of Boron Modifications of Palladium Catalysts for the Production of Hydrogen from Formic Acid. <i>ACS Catalysis</i> , 2015 , 5, 6579-6586	13.1	68
22	Propane Dehydrogenation over Pt/TiO ₂ /Al ₂ O ₃ Catalysts. <i>ACS Catalysis</i> , 2015 , 5, 438-447	13.1	177
21	Mechanistic Understanding of the Plasmonic Enhancement for Solar Water Splitting. <i>Advanced Materials</i> , 2015 , 27, 5328-42	24	301
20	Molecular understandings on the activation of light hydrocarbons over heterogeneous catalysts. <i>Chemical Science</i> , 2015 , 6, 4403-4425	9.4	141
19	Sub-10 nm rutile titanium dioxide nanoparticles for efficient visible-light-driven photocatalytic hydrogen production. <i>Nature Communications</i> , 2015 , 6, 5881	17.4	535
18	Exceptional size-dependent activity enhancement in the electroreduction of CO ₂ over Au nanoparticles. <i>Journal of the American Chemical Society</i> , 2014 , 136, 16473-6	16.4	495
17	First-principles analysis of defect-mediated Li adsorption on graphene. <i>ACS Applied Materials & Interfaces</i> , 2014 , 6, 21141-50	9.5	92
16	Propane dehydrogenation over Pt-Cu bimetallic catalysts: the nature of coke deposition and the role of copper. <i>Nanoscale</i> , 2014 , 6, 10000-8	7.7	146
15	Reactivity of the Defective Rutile TiO ₂ (110) Surfaces with Two Bridging-Oxygen Vacancies: Water Molecule as a Probe. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 20257-20263	3.8	16
14	Controllable fabrication of nanostructured materials for photoelectrochemical water splitting via atomic layer deposition. <i>Chemical Society Reviews</i> , 2014 , 43, 7469-84	58.5	187
13	Dendritic Au/TiO ₂ nanorod arrays for visible-light driven photoelectrochemical water splitting. <i>Nanoscale</i> , 2013 , 5, 9001-9	7.7	211
12	Formation of n-hexane from methylcyclopentane via a metallacyclobutane intermediate at step sites of Pt surfaces: Mechanism from first-principles calculations. <i>Journal of Catalysis</i> , 2013 , 299, 146-149	7.3	10

11	Ring-Opening Reactions of Methylcyclopentane over Metal Catalysts, M = Pt, Rh, Ir, and Pd: A Mechanistic Study from First-Principles Calculations. <i>ACS Catalysis</i> , 2013 , 3, 196-205	13.1	33
10	Tuning the selectivity for ring-opening reactions of methylcyclopentane over Pt catalysts: A mechanistic study from first-principles calculations. <i>Journal of Catalysis</i> , 2012 , 285, 124-133	7.3	38
9	Ethylene conversion to ethylidyne on Pd(111) and Pt(111): A first-principles-based kinetic Monte Carlo study. <i>Journal of Catalysis</i> , 2012 , 285, 187-195	7.3	61
8	Theoretical study on the leaching of palladium in a CO atmosphere. <i>Catalysis Science and Technology</i> , 2012 , 2, 2238	5.5	17
7	Recent advances in catalytic hydrogenation of carbon dioxide. <i>Chemical Society Reviews</i> , 2011 , 40, 3703-3755	22	16
6	Decomposition of ethylene on transition metal surfaces M(111). A comparative DFT study of model reactions for M=Pd, Pt, Rh, Ni. <i>Journal of Molecular Catalysis A</i> , 2011 , 344, 37-46		48
5	Ethylidyne Formation from Ethylene over Pt(111): A Mechanistic Study from First-Principle Calculations. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 12190-12201	3.8	71
4	Ethylidyne Formation from Ethylene over Pd(111): Alternative Routes from a Density Functional Study. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 15373-15379	3.8	28
3	Structured water and water-polymer interactions in hydrogels of molecularly imprinted polymers. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 7515-21	3.4	27
2	Size effect on competition of two diffusion mechanisms for drug molecules in amorphous polymers. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 13167-72	3.4	9
1	A different diffusion mechanism for drug molecules in amorphous polymers. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 4411-6	3.4	18