Xue-Qing Gong

List of Publications by Citations

215 papers	9,688 citations	55 h-index	92 g-index
231 ext. papers	11,327 ext. citations	8.5 avg, IF	6.53 L-index

#	Paper	IF	Citations
215	Reactivity of anatase TiO(2) nanoparticles: the role of the minority (001) surface. *Journal of Physical Chemistry B*, **2005**, 109, 19560-2	3.4	543
214	Catalytic role of metal oxides in gold-based catalysts: a first principles study of CO oxidation on TiO2 supported Au. *Physical Review Letters*, **2003**, 91, 266102	7.4	358
213	Steps on anatase TiO2(101). *Nature Materials*, **2006**, 5, 665-70	27	357
212	Boosting power conversion efficiencies of quantum-dot-sensitized solar cells beyond 8% by recombination control. *Journal of the American Chemical Society*, **2015**, 137, 5602-9	16.4	330
211	Direct hydrodeoxygenation of raw woody biomass into liquid alkanes. *Nature Communications*, **2016**, 7, 11162	17.4	271
210	Small Au and Pt clusters at the anatase TiO2(101) surface: behavior at terraces, steps, and surface oxygen vacancies. *Journal of the American Chemical Society*, **2008**, 130, 370-81	16.4	254
209	Ultrathin Metal-Organic Framework Nanosheets with Ultrahigh Loading of Single Pt Atoms for Efficient Visible-Light-Driven Photocatalytic H Evolution. *Angewandte Chemie - International Edition*, **2019**, 58, 10198-10203	16.4	239
208	A systematic study of CO oxidation on metals and metal oxides: density functional theory calculations. *Journal of the American Chemical Society*, **2004**, 126, 8-9	16.4	238
207	On the Unusual Properties of Anatase TiO2 Exposed by Highly Reactive Facets. *Journal of Physical Chemistry Letters*, **2011**, 2, 725-734	6.4	211
206	Pd/NbOPO□multifunctional catalyst for the direct production of liquid alkanes from aldol adducts of furans. *Angewandte Chemie - International Edition*, **2014**, 53, 9755-60	16.4	207
205	Multiple configurations of the two excess 4f electrons on defective CeO2(111): Origin and implications. *Physical Review B*, **2009**, 79,	3.3	202
204	Density functional theory study of formic acid adsorption on anatase TiO2(001): geometries, energetics, and effects of coverage, hydration, and reconstruction. *Journal of Physical Chemistry B*, **2006**, 110, 2804-11	3.4	200
203	Hydrogen bonding controls the dynamics of catechol adsorbed on a TiO2(110) surface. *Science*, **2010**, 328, 882-4	33.3	193
202	An efficiently tuned d-orbital occupation of IrO by doping with Cu for enhancing the oxygen evolution reaction activity. *Chemical Science*, **2015**, 6, 4993-4999	9.4	146
201	Anatase TiO2 crystals with exposed high-index facets. *Angewandte Chemie - International Edition*, **2011**, 50, 3764-8	16.4	142
200	Boosting Interfacial Charge-Transfer Kinetics for Efficient Overall CO Photoreduction via Rational Design of Coordination Spheres on Metal-Organic Frameworks. *Journal of the American Chemical Society*, **2020**, 142, 12515-12523	16.4	131
199	Effect of the crystal plane figure on the catalytic performance of MnO2 for the total oxidation of propane. *CrystEngComm*, **2015**, 17, 3005-3014	3.3	125

198	Molecular Engineering of Donor–Acceptor Conjugated Polymer/g-C3N4 Heterostructures for Significantly Enhanced Hydrogen Evolution Under Visible-Light Irradiation. *Advanced Functional Materials*, **2018**, 28, 1804512	15.6	115
197	Taming the stability of Pd active phases through a compartmentalizing strategy toward nanostructured catalyst supports. *Nature Communications*, **2019**, 10, 1611	17.4	112
196	CO dissociation and O removal on Co(0001): a density functional theory study. *Surface Science*, **2004**, 562, 247-256	1.8	112
195	C NMR guides rational design of nanocatalysts via chemisorption evaluation in liquid phase. *Science*, **2011**, 332, 224-8	33.3	106
194	An Artificial Molecular Shuttle Operates in Lipid Bilayers for Ion Transport. *Journal of the American Chemical Society*, **2018**, 140, 17992-17998	16.4	104
193	The catalytic role of water in CO oxidation. *Journal of Chemical Physics*, **2003**, 119, 6324-6334	3.9	102
192	Enhanced Photocatalysis by Au Nanoparticle Loading on TiO2 Single-Crystal (001) and (110) Facets. *Journal of Physical Chemistry Letters*, **2013**, 4, 3910-3917	6.4	99
191	Prominent electronic and geometric modifications of palladium nanoparticles by polymer stabilizers for hydrogen production under ambient conditions. *Angewandte Chemie - International Edition*, **2012**, 51, 11275-8	16.4	99
190	A Model to Understand the Oxygen Vacancy Formation in Zr-Doped CeO2: Electrostatic Interaction and Structural Relaxation. *Journal of Physical Chemistry C*, **2009**, 113, 10229-10232	3.8	97
189	The 2 reconstruction of the rutile TiO2(011) surface: A combined density functional theory, X-ray diffraction, and scanning tunneling microscopy study. *Surface Science*, **2009**, 603, 138-144	1.8	96
188	First-principles study of the structures and energetics of stoichiometric brookite TiO2 surfaces. *Physical Review B*, **2007**, 76,	3.3	88
187	Current status and perspectives of rare earth catalytic materials and catalysis. *Chinese Journal of Catalysis*, **2014**, 35, 1238-1250	11.3	87
186	Different Reactivities of TiO2Polymorphs: Comparative DFT Calculations of Water and Formic Acid Adsorption at Anatase and Brookite TiO2Surfaces. *Journal of Physical Chemistry C*, **2008**, 112, 6594-6596	3.8	84
185	CHx hydrogenation on Co(0001): a density functional theory study. *Journal of Chemical Physics*, **2005**, 122, 024711	3.9	84
184	Evidence to challenge the universality of the Horiuti-Polanyi mechanism for hydrogenation in heterogeneous catalysis: origin and trend of the preference of a non-Horiuti-Polanyi mechanism. *Journal of the American Chemical Society*, **2013**, 135, 15244-50	16.4	83
183	Oxygen vacancies induced visible-light photocatalytic activities of CaCu3Ti4O12 with controllable morphologies for antibiotic degradation. *Applied Catalysis B: Environmental*, **2018**, 221, 422-432	21.8	80
182	Photocatalytic reduction of CO2 with water vapor on surface La-modified TiO2 nanoparticles with enhanced CH4 selectivity. *Applied Catalysis B: Environmental*, **2015**, 168-169, 125-131	21.8	77
181	Study of Catalytic Sites on Ruthenium For Hydrogenation of N-ethylcarbazole: Implications of Hydrogen Storage via Reversible Catalytic Hydrogenation. *Journal of Physical Chemistry C*, **2010**, 114, 9720-9730	3.8	76

180	Interfacial Effects of CeO2-Supported Pd Nanorod in Catalytic CO Oxidation: A Theoretical Study. *Journal of Physical Chemistry C*, **2015**, 119, 12923-12934	3.8	71
179	Oxygen vacancy formation in CeO2 and Ce(1-x)Zr(x)O2 solid solutions: electron localization, electrostatic potential and structural relaxation. *Physical Chemistry Chemical Physics*, **2012**, 14, 16521-35	3.6	71
178	Role of steps in the reactivity of the anatase TiO2(101) surface. *Journal of Catalysis*, **2007**, 249, 134-139	7.3	67
177	Study on the catalytic reaction mechanism of low temperature oxidation of CO over Pd□Cu□Clx/Al2O3 catalyst. *Catalysis Today*, **2011**, 175, 558-567	5.3	64
176	Mechanistic Study of Selective Catalytic Reduction of NO with NH3 on W-Doped CeO2 Catalysts: Unraveling the Catalytic Cycle and the Role of Oxygen Vacancy. *Journal of Physical Chemistry C*, **2016**, 120, 2271-2283	3.8	63
175	Layered nanostructured ferroelectric perovskite Bi5FeTi3O15 for visible light photodegradation of antibiotics. *Journal of Materials Chemistry A*, **2017**, 5, 21275-21290	13	63
174	Role and reduction of NOx in the catalytic combustion of soot over iron□ceria mixed oxide catalyst. *Chemical Engineering Journal*, **2013**, 218, 164-172	14.7	62
173	A DFT+U study of the lattice oxygen reactivity toward direct CO oxidation on the CeO2(111) and (110) surfaces. *Physical Chemistry Chemical Physics*, **2012**, 14, 16573-80	3.6	62
172	A highly effective catalyst of Co-CeO 2 for the oxidation of diesel soot: The excellent NO oxidation activity and NO x storage capacity. *Applied Catalysis A: General*, **2017**, 535, 1-8	5.1	61
171	Catalytic total oxidation of 1,2-dichloroethane over VO x /CeO 2 catalysts: Further insights via isotopic tracer techniques. *Applied Catalysis B: Environmental*, **2016**, 182, 598-610	21.8	61
170	OER activity manipulated by IrO coordination geometry: an insight from pyrochlore iridates. *Scientific Reports*, **2016**, 6, 38429	4.9	60
169	Shape Effect of Pd-Promoted Ga2O3 Nanocatalysts for Methanol Synthesis by CO2 Hydrogenation. *Journal of Physical Chemistry C*, **2014**, 118, 24452-24466	3.8	59
168	Hollandite Structure K(x□.25)IrO2 Catalyst with Highly Efficient Oxygen Evolution Reaction. *ACS Applied Materials & Interfaces*, **2016**, 8, 820-6	9.5	58
167	Ni□Co Codoping Breaks the Limitation of Single-Metal-Doped IrO2 with Higher Oxygen Evolution Reaction Performance and Less Iridium. *ACS Energy Letters*, **2017**, 2, 2786-2793	20.1	57
166	Role of oxygen vacancies in the surface evolution of H at CeO2(111): a charge modification effect. *Physical Chemistry Chemical Physics*, **2015**, 17, 3544-9	3.6	57
165	The Critical Role of Water in the Ring Opening of Furfural Alcohol to 1,2-Pentanediol. *ACS Catalysis*, **2017**, 7, 333-337	13.1	56
164	Ultrathin Metal□Organic Framework Nanosheets with Ultrahigh Loading of Single Pt Atoms for Efficient Visible-Light-Driven Photocatalytic H2 Evolution. *Angewandte Chemie*, **2019**, 131, 10304-10309	3.6	56
163	A promising low pressure methanol synthesis route from CO2 hydrogenation over Pd@Zn core□shell catalysts. *Green Chemistry*, **2017**, 19, 270-280	10	56

162	Formation of New Structures and Their Synergistic Effects in Boron and Nitrogen Codoped TiO2 for Enhancement of Photocatalytic Performance. *Journal of Physical Chemistry C*, **2011**, 115, 7858-7865	3.8	56
161	Realizing highly chemoselective detection of HS in vitro and in vivo with fluorescent probes inside core-shell silica nanoparticles. *Biomaterials*, **2018**, 159, 82-90	15.6	55
160	Polymer-templated synthesis of hollow Pd CeO2 nanocomposite spheres and their catalytic activity and thermal stability. *Journal of Materials Chemistry A*, **2015**, 3, 23230-23239	13	54
159	Methanol Conversion into Dimethyl Ether on the Anatase TiO2(001) Surface. *Angewandte Chemie - International Edition*, **2016**, 55, 623-8	16.4	54
158	Effects of Metal Oxyhydroxide Coatings on Photoanode in Quantum Dot Sensitized Solar Cells. *Chemistry of Materials*, **2016**, 28, 2323-2330	9.6	53
157	Identification of different oxygen species in oxide nanostructures with (17)O solid-state NMR spectroscopy. *Science Advances*, **2015**, 1, e1400133	14.3	53
156	CO Oxidation at Rutile TiO2(110): Role of Oxygen Vacancies and Titanium Interstitials. *ACS Catalysis* , **2015**, 5, 2042-2050	13.1	53
155	A density functional theory study of hydrogen dissociation and diffusion at the perimeter sites of Au/TiO2. *Physical Chemistry Chemical Physics*, **2012**, 14, 3741-5	3.6	51
154	Effect of lattice strain on the electro-catalytic activity of IrO for water splitting. *Chemical Communications*, **2018**, 54, 996-999	5.8	50
153	A density functional theory study of small Au nanoparticles at CeO2 surfaces. *Catalysis Today*, **2011**, 165, 19-24	5.3	47
152	Acrolein hydrogenation on Pt(211) and Au(211) surfaces: a density functional theory study. *Physical Chemistry Chemical Physics*, **2011**, 13, 21146-52	3.6	46
151	Clustering of Oxygen Vacancies at CeO2(111): Critical Role of Hydroxyls. *Physical Review Letters*, **2016**, 116, 086102	7.4	45
150	Operando NMR spectroscopic analysis of proton transfer in heterogeneous photocatalytic reactions. *Nature Communications*, **2016**, 7, 11918	17.4	43
149	High-performance PdNi alloy structured in situ on monolithic metal foam for coalbed methane deoxygenation via catalytic combustion. *Chemical Communications*, **2015**, 51, 12613-6	5.8	41
148	Size-dependent catalytic performance of ruthenium nanoparticles in the hydrogenolysis of a O-4 lignin model compound. *Catalysis Science and Technology*, **2018**, 8, 735-745	5.5	41
147	General insight into CO oxidation: a density functional theory study of the reaction mechanism on platinum oxides. *Physical Review Letters*, **2004**, 93, 106104	7.4	41
146	A DFT+U study of CO oxidation at CeO2(110) and (111) surfaces with oxygen vacancies. *Surface Science*, **2013**, 618, 140-147	1.8	39
145	Diffusion and Reaction of Hydrogen on Rutile TiO2(011)-2 1: The Role of Surface Structure. *Journal of Physical Chemistry C*, **2012**, 116, 20438-20446	3.8	39

144	Distinguishing faceted oxide nanocrystals with O solid-state NMR spectroscopy. *Nature Communications*, **2017**, 8, 581	17.4	38
143	Unique Electronic and Structural Effects in Vanadia/Ceria-Catalyzed Reactions. *Journal of the American Chemical Society*, **2015**, 137, 13228-31	16.4	37
142	Mechanism of CO2 Photocatalytic Reduction to Methane and Methanol on Defected Anatase TiO2 (101): A Density Functional Theory Study. *Journal of Physical Chemistry C*, **2019**, 123, 3505-3511	3.8	36
141	Cooperative catalysis for the direct hydrodeoxygenation of vegetable oils into diesel-range alkanes over Pd/NbOPO4. *Chemical Communications*, **2016**, 52, 5160-3	5.8	34
140	Trapping Nitric Oxide by Surface Hydroxyls on Rutile TiO2(110). *Journal of Physical Chemistry C*, **2012**, 116, 1887-1891	3.8	32
139	Nucleation and Growth of 1D Water Clusters on Rutile TiO2 (011)-2□1. *Journal of Physical Chemistry C*, **2009**, 113, 10329-10332	3.8	32
138	Octahedral-shaped perovskite CaCu3Ti4O12 with dual defects and coexposed {(001), (111)} facets for visible-light photocatalysis. *Applied Catalysis B: Environmental*, **2019**, 254, 86-97	21.8	31
137	Structure and Catalytic Activity of Gold in Low-Temperature CO Oxidation. *Journal of Physical Chemistry C*, **2009**, 113, 6124-6131	3.8	31
136	Surface Reconstruction-Induced Site-Specific Charge Separation and Photocatalytic Reaction on Anatase TiO2(001) Surface. *Journal of Physical Chemistry C*, **2017**, 121, 9991-9999	3.8	30
135	Fluorinated conjugated poly(benzotriazole)/g-C3N4 heterojunctions for significantly enhancing photocatalytic H2 evolution. *Applied Catalysis B: Environmental*, **2020**, 267, 118577	21.8	30
134	High-Performance PdNi Nanoalloy Catalyst in Situ Structured on Ni Foam for Catalytic Deoxygenation of Coalbed Methane: Experimental and DFT Studies. *ACS Catalysis*, **2016**, 6, 6236-6245	13.1	30
133	High Performance and Stability of the Pt-W/ZSM-5 Catalyst for the Total Oxidation of Propane: The Role of Tungsten. *ChemCatChem*, **2013**, 5, 2495-2503	5.2	30
132	N-Annulated perylene-based organic dyes sensitized graphitic carbon nitride to form an amide bond for efficient photocatalytic hydrogen production under visible-light irradiation. *Applied Catalysis B: Environmental*, **2018**, 237, 32-42	21.8	30
131	A highly effective Ni-modified MnOx catalyst for total oxidation of propane: the promotional role of nickel oxide. *RSC Advances*, **2016**, 6, 50228-50237	3.7	29
130	AgBr tetradecahedrons with co-exposed {100} and {111} facets: simple fabrication and enhancing spatial charge separation using facet heterojunctions. *Journal of Materials Chemistry A*, **2016**, 4, 18570-18577	13	29
129	Catalytic Activity Control via Crossover between Two Different Microstructures. *Journal of the American Chemical Society*, **2017**, 139, 13740-13748	16.4	29
128	Preparation, characterization and origin of highly active and thermally stable Pd-Ce0.8Zr0.2O2 catalysts via sol-evaporation induced self-assembly method. *Environmental Science & Technology*, **2014**, 48, 12403-10	10.3	29
127	New directions for atomic steps: step alignment by grazing incident ion beams on TiO2(110). *Physical Review Letters*, **2009**, 102, 166103	7.4	29

126	Mechanism of Surface-Enhanced Raman Scattering Based on 3D Graphene-TiO Nanocomposites and Application to Real-Time Monitoring of Telomerase Activity in Differentiation of Stem Cells. *ACS Applied Materials & Interfaces*, **2017**, 9, 36596-36605	9.5	28
125	Facet-dependent photocatalytic performance of TiO 2 : A DFT study. *Applied Catalysis B: Environmental*, **2016**, 198, 1-8	21.8	28
124	Methanol Synthesis at a Wide Range of H /CO Ratios over a Rh-In Bimetallic Catalyst. *Angewandte Chemie - International Edition*, **2020**, 59, 16039-16046	16.4	27
123	Elucidation of the high CO2 reduction selectivity of isolated Rh supported on TiO2: a DFT study. *Catalysis Science and Technology*, **2016**, 6, 6128-6136	5.5	27
122	A highly-efficient LaMnOx catalyst for propane combustion: the promotional role of La and the effect of the preparation method. *Catalysis Science and Technology*, **2016**, 6, 8222-8233	5.5	26
121	Chemical activity of oxygen vacancies on ceria: a combined experimental and theoretical study on CeO2(111). *Physical Chemistry Chemical Physics*, **2014**, 16, 24165-8	3.6	26
120	Polar surface structure of oxide nanocrystals revealed with solid-state NMR spectroscopy. *Nature Communications*, **2019**, 10, 5420	17.4	26
119	Synthesis of a hollow structured coreshell Au@CeO2ZrO2 nanocatalyst and its excellent catalytic performance. *Journal of Materials Chemistry A*, **2017**, 5, 5601-5611	13	25
118	Origin of the High Activity of Mesoporous CeO2 Supported Monomeric VOx for Low-Temperature Gas-Phase Selective Oxidative Dehydrogenation of Benzyl Alcohol: Role As an Electronic Hole *Journal of Physical Chemistry C*, **2014**, 118, 24950-24958	3.8	25
117	Adsorbate induced restructuring of TiO2(011)-(21) leads to one-dimensional nanocluster formation. *Physical Review Letters*, **2012**, 108, 106105	7.4	25
116	(Photo)Electrocatalytic CO2 Reduction at the Defective Anatase TiO2 (101) Surface. *ACS Catalysis*, **2020**, 10, 4048-4058	13.1	24
115	Pt-Doped NiFeO Spinel as a Highly Efficient Catalyst for H Selective Catalytic Reduction of NO at Room Temperature. *ACS Combinatorial Science*, **2016**, 18, 195-202	3.9	24
114	Brsted base site engineering of graphitic carbon nitride for enhanced photocatalytic activity. *Journal of Materials Chemistry A*, **2017**, 5, 19227-19236	13	24
113	Strategies To Improve the Activity While Maintaining the Selectivity of Oxidative Coupling of Methane at La2O3: A Density Functional Theory Study. *ACS Catalysis*, **2020**, 10, 586-594	13.1	24
112	Localized Electrons Enhanced Ion Transport for Ultrafast Electrochemical Energy Storage. *Advanced Materials*, **2020**, 32, e1905578	24	23
111	The stability and deactivation of PdCuClx/Al2O3 catalyst for low temperature CO oxidation: an effect of moisture. *Catalysis Science and Technology*, **2011**, 1, 1202	5.5	23
110	Metal-Free Ceria Catalysis for Selective Hydrogenation of Crotonaldehyde. *ACS Catalysis*, **2020**, 10, 14560-14566	13.1	23
109	Dispersed Nickel Boosts Catalysis by Copper in CO2 Hydrogenation. *ACS Catalysis*, **2020**, 10, 9261-9270	13.1	23

108	A DFT + U study of V, Cr and Mn doped CeO2(111). *Applied Surface Science*, **2018**, 428, 377-384	6.7	22
107	Function-oriented design of robust metal cocatalyst for photocatalytic hydrogen evolution on metal/titania composites. *Nature Communications*, **2021**, 12, 158	17.4	22
106	Enhancing photocatalytic activity of Sn doped TiO2 dominated with {1 0 5} facets. *Catalysis Today*, **2014**, 225, 18-23	5.3	21
105	Anatase TiO2 Crystals with Exposed High-Index Facets. *Angewandte Chemie*, **2011**, 123, 3848-3852	3.6	21
104	A density functional theory study on the water formation at high coverages and the water effect in the Fischer□ropsch synthesis. *Molecular Physics*, **2004**, 102, 993-1000	1.7	21
103	Catalytic activities of CeO2(110)□ □ reconstructed surface. *Surface Science*, **2015**, 632, 164-173	1.8	19
102	A comparative DFT study of adsorption and catalytic performance of Au nanoparticles at anatase and brookite TiO2 surfaces. *Surface Science*, **2011**, 605, 1369-1380	1.8	19
101	Site Sensitivity of Interfacial Charge Transfer and Photocatalytic Efficiency in Photocatalysis: Methanol Oxidation on Anatase TiO Nanocrystals. *Angewandte Chemie - International Edition*, **2021**, 60, 6160-6169	16.4	18
100	Selective hydrogenation of 5-(hydroxymethyl)furfural to 5-methylfurfural over single atomic metals anchored on NbO. *Nature Communications*, **2021**, 12, 584	17.4	18
99	Methanol Dynamically Activated Room-Temperature Phosphorescence from a Twisted 4-Bromobiphenyl System. *CCS Chemistry*, **2020**, 2, 158-167	7.2	17
98	Superior Performance of Ag over Pt for Hydrogen Evolution Reaction in Water Electrolysis under High Overpotentials. *ACS Applied Energy Materials*, **2019**, 2, 1221-1228	6.1	16
97	Unique adsorption behaviors of carboxylic acids at rutile TiO2(110). *Surface Science*, **2015**, 641, 82-90	1.8	16
96	Solvent-free selective oxidation of cyclohexane with molecular oxygen over manganese oxides: Effect of the calcination temperature. *Chinese Journal of Catalysis*, **2016**, 37, 184-192	11.3	16
95	Interaction of Hydrogen with Ceria: Hydroxylation, Reduction, and Hydride Formation on the Surface and in the Bulk. *Chemistry - A European Journal*, **2021**, 27, 5268-5276	4.8	16
94	Ligand-mediated bifunctional catalysis for enhanced oxygen reduction and methanol oxidation tolerance in fuel cells. *Journal of Materials Chemistry A*, **2018**, 6, 18884-18890	13	16
93	Ionic Liquid Stabilized Niobium Oxoclusters Catalyzing Oxidation of Sulfides with Exceptional Activity. *Chemistry - A European Journal*, **2019**, 25, 4206-4217	4.8	15
92	Tailoring nano-catalysts: turning gold nanoparticles on bulk metal oxides to inverse nano-metal oxides on large gold particles. *Chemical Communications*, **2015**, 51, 5975-8	5.8	15
91	Surfactant-Mediated One-Pot Method To Prepare Pd-CeO Colloidal Assembled Spheres and Their Enhanced Catalytic Performance for CO Oxidation. *ACS Omega*, **2016**, 1, 118-126	3.9	15

90	Identification of different tin species in SnO2 nanosheets with 119Sn solid-state NMR spectroscopy. *Chemical Physics Letters*, **2016**, 643, 126-130	2.5	15
89	Catalytic properties of Pt/Al2O3 catalysts in the aqueous-phase reforming of ethylene glycol: Effect of the alumina support. *Kinetics and Catalysis*, **2011**, 52, 817-822	1.5	15
88	Pd@Zn core–shell nanoparticles of controllable shell thickness for catalytic methanol production. *Catalysis Science and Technology*, **2016**, 6, 7698-7702	5.5	15
87	17O Solid-State NMR Studies of ZrO2 Nanoparticles. *Journal of Physical Chemistry C*, **2019**, 123, 4158-4167	3.8	14
86	A promising engineering strategy for water electro-oxidation iridate catalysts via coordination distortion. *Chemical Communications*, **2019**, 55, 5801-5804	5.8	14
85	Prediction of Ir0.5M0.5O2 (M = Cr, Ru or Pb) Mixed Oxides as Active Catalysts for Oxygen Evolution Reaction from First-Principles Calculations. *Topics in Catalysis*, **2015**, 58, 675-681	2.3	14
84	NO adsorption and diffusion on hydroxylated rutile TiO2(110). *Physical Chemistry Chemical Physics*, **2015**, 17, 26594-8	3.6	14
83	The synthesis of Co-doped SAPO-5 molecular sieve and its performance in the oxidation of cyclohexane with molecular oxygen. *Chinese Journal of Catalysis*, **2016**, 37, 273-280	11.3	13
82	Activity and selectivity of propane oxidative dehydrogenation over VO3/CeO2(111) catalysts: A density functional theory study. *Chinese Journal of Catalysis*, **2018**, 39, 1520-1526	11.3	13
81	Selective tracking of ovarian-cancer-specific γ-glutamyltranspeptidase using a ratiometric two-photon fluorescent probe. *Journal of Materials Chemistry B*, **2018**, 6, 7439-7443	7.3	13
80	Ordered Fe(II)Ti(IV)O3 Mixed Monolayer Oxide on Rutile TiO2(011). *ACS Nano*, **2015**, 9, 8627-36	16.7	12
79	Interactions of Oxide Surfaces with Water Revealed with Solid-State NMR Spectroscopy. *Journal of the American Chemical Society*, **2020**, 142, 11173-11182	16.4	12
78	A DFT + U study of NO evolution at reduced CeO2(110). *Physical Chemistry Chemical Physics*, **2014**, 16, 16904-8	3.6	12
77	Hydrodeoxygenation of butyric acid at multi-functional Nb2O5 catalyst: A density functional theory study. *International Journal of Hydrogen Energy*, **2016**, 41, 18502-18508	6.7	12
76	Preparation of lamellar-stacked TS-1 and its catalytic performance for the ammoximation of butanone with H2O2. *Journal of Materials Science*, **2018**, 53, 4034-4045	4.3	12
75	A DFT+U study of the catalytic degradation of 1,2-dichloroethane over CeO. *Physical Chemistry Chemical Physics*, **2018**, 20, 5856-5864	3.6	11
74	Promotional Effect of Carbon on Fe Catalysts for Ammonia Decomposition: A Density Functional Theory Study. *Industrial & Engineering Chemistry Research*, **2013**, 52, 17151-17155	3.9	11
73	A DFT study on surface dependence of γ-Ga2O 3 for CO 2 hydrogenation to CH 3OH. *Journal of Molecular Modeling*, **2014**, 20, 2543	2	11

72	Unique adsorption behaviors of NO and O2 at hydrogenated anatase TiO2(101). *Chinese Chemical Letters*, **2018**, 29, 765-768	8.1	10
71	Monolayer Intermixed Oxide Surfaces: Fe, Ni, Cr, and V Oxides on Rutile TiO2(011). *Journal of Physical Chemistry C*, **2016**, 120, 14782-14794	3.8	10
70	Effect of One-Pot Rehydration Process on Surface Basicity and Catalytic Activity of MgyAl1-aREEaOx Catalyst for Aldol Condensation of Citral and Acetone. *ACS Sustainable Chemistry and Engineering*, **2016**, 4, 1591-1601	8.3	10
69	A DFT+U revisit of reconstructed CeO(100) surfaces: structures, thermostabilities and reactivities. *Physical Chemistry Chemical Physics*, **2019**, 21, 19987-19994	3.6	10
68	Combined Surface Science and DFT Study of the Adsorption of Dinitrotoluene (2,4-DNT) on Rutile TiO2(110): Molecular Scale Insight into Sensing of Explosives. *Journal of Physical Chemistry C*, **2013**, 117, 16468-16476	3.8	10
67	Bandgap engineering of novel peryleno[1,12-bcd]thiophene sulfone-based conjugated co-polymers for significantly enhanced hydrogen evolution without co-catalyst. *Journal of Materials Chemistry A*, **2020**, 8, 20062-20071	13	10
66	Construction of polymeric carbon nitride and dibenzothiophene dioxide-based intramolecular donor–acceptor conjugated copolymers for photocatalytic H2 evolution. *Nanoscale Advances*, **2021**, 3, 1699-1707	5.1	10
65	A new PET and FRET-based molecular logic circuit mimicking the three-state logic gate. *Dyes and Pigments*, **2017**, 140, 460-468	4.6	9
64	Anatase TiO2(001)-(1 × 4) Surface Is Intrinsically More Photocatalytically Active than the Rutile TiO2(110)-(1 × 1) Surface. *Journal of Physical Chemistry C*, **2019**, 123, 24558-24565	3.8	9
63	Density functional theory study of mixed-phase TiO₂ heterostructures and electronic properties. *Journal of Molecular Modeling*, **2014**, 20, 2215	2	9
62	Methanol Conversion into Dimethyl Ether on the Anatase TiO2(001) Surface. *Angewandte Chemie*, **2016**, 128, 633-638	3.6	9
61	Room temperature efficient reduction of NOx by H2 in a permeable compounded membrane – Catalytic reactor. *Chemical Engineering Journal*, **2016**, 283, 929-935	14.7	8
60	More than oxygen vacancies: a collective crystal-plane effect of CeO2 in gas-phase selective oxidation of benzyl alcohol. *Catalysis Science and Technology*, **2019**, 9, 2960-2967	5.5	8
59	Influence of Cl substitution on the electronic structure and catalytic activity of ceria. *Science China Chemistry*, **2015**, 58, 601-606	7.9	8
58	DFT + U study of the CO + NOx reaction on a CeO2(110)-supported Au nanoparticle. *Chinese Journal of Catalysis*, **2014**, 35, 1305-1317	11.3	8
57	Dendrimer-mediated hydrothermal synthesis of ultrathin gold nanowires. *Scientific Reports*, **2013**, 3, 3181	4.9	8
56	Selectivity switching resulting in the formation of benzene by surface carbonates on ceria in catalytic gas-phase oxidation of benzyl alcohol. *Chemical Communications*, **2016**, 52, 2827-30	5.8	7
55	A DFT study of the CO adsorption and oxidation at ZnO surfaces and its implication for CO detection. *Chinese Chemical Letters*, **2020**, 31, 1674-1679	8.1	7

54	A DFT+U study on the oxidative chlorination of CH4 at ceria: the role of HCl. *Catalysis Science and Technology*, **2017**, 7, 2498-2505	5.5	6
53	Gas phase selective propylene epoxidation over La2O3-supported cubic silver nanoparticles. *Catalysis Science and Technology*, **2019**, 9, 3435-3444	5.5	6
52	Theoretical studies on the monomeric vanadium oxides supported by ceria: the atomic structures and oxidative dehydrogenation activities. *RSC Advances*, **2015**, 5, 52259-52263	3.7	6
51	Strategies of alloying effect for regulating Pt-based H-SCR catalytic activity. *Chemical Communications*, **2018**, 54, 9502-9505	5.8	6
50	A DFT+U study of the structures and reactivities of polar CeO2(100) surfaces. *Chinese Journal of Catalysis*, **2017**, 38, 1138-1147	11.3	6
49	Genetic algorithm aided density functional theory simulations unravel the kinetic nature of Au(100) in catalytic CO oxidation. *Chinese Chemical Letters*, **2019**, 30, 1346-1350	8.1	6
48	Realization approach of Pd-only three-way catalysts with high catalytic performance and thermal stability. *Science China Chemistry*, **2015**, 58, 123-130	7.9	5
47	Clarifying the impacts of surface hydroxyls on CO oxidation on CeO(100) surfaces: a DFT+U study. *Physical Chemistry Chemical Physics*, **2020**, 22, 7738-7746	3.6	5
46	N-doped graphitic CN nanosheets decorated with CoP nanoparticles: A highly efficient activator in singlet oxygen dominated visible-light-driven peroxymonosulfate activation for degradation of pharmaceuticals and personal care products. *Journal of Hazardous Materials*, **2021**, 416, 125891	12.8	5
45	An Ordered Mixed Oxide Monolayer Formed by Iron Segregation on Rutile-TiO2(011): Structural Determination by X-ray Photoelectron Diffraction. *Journal of Physical Chemistry C*, **2016**, 120, 26414-26424	3.8	4
44	A mechanistic study of syngas conversion to light olefins over OXZEO bifunctional catalysts: insights into the initial carbon–carbon bond formation on the oxide. *Catalysis Science and Technology*,	5.5	4
43	Fe(II)Ti(IV)O3 mixed oxide monolayer at rutile TiO2(011): Structures and reactivities. *Surface Science*, **2016**, 653, 34-40	1.8	4
42	Reactions of Molten LiI with I2, H2O, and O2 Relevant to Halogen-Mediated Oxidative Dehydrogenation of Alkanes. *Journal of Physical Chemistry C*, **2016**, 120, 4931-4936	3.8	4
41	Site Sensitivity of Interfacial Charge Transfer and Photocatalytic Efficiency in Photocatalysis: Methanol Oxidation on Anatase TiO2 Nanocrystals. *Angewandte Chemie*, **2021**, 133, 6225-6234	3.6	4
40	Efficient and stable photocatalytic H2 evolution by self-assembly of zirconium(IV) coordination with perylene diimide supramolecules under visible light irradiation. *Journal of Materials Chemistry A*, **2021**, 9, 7675-7683	13	4
39	Core-Shell Nanostructured Ru@Ir-O Electrocatalysts for Superb Oxygen Evolution in Acid.. *Small*, **2022**, e2108031	11	4
38	Methanol Synthesis at a Wide Range of H2/CO2 Ratios over a Rh-In Bimetallic Catalyst. *Angewandte Chemie*, **2020**, 132, 16173-16180	3.6	3
37	Computational Simulation of Rare Earth Catalysis. *Advances in Chemical Engineering*, **2014**, 1-60	0.6	3

36	FeOOH photo-deposited perylene linear polymer with accelerated charge separation for photocatalytic overall water splitting. *Science China Chemistry*, **2022**, 65, 170	7.9	3
35	Trace of molecular doping in metal–organic frameworks: drastic change in the electronic band structure with a preserved topology and porosity. *Journal of Materials Chemistry A*, **2020**, 8, 12370-12377	13	3
34	Structures and reactivities of the CeO2/Pt(111) reverse catalyst: A DFT+U study. *Chinese Journal of Catalysis*, **2020**, 41, 1360-1368	11.3	3
33	Ionic liquid-stabilized vanadium oxo-clusters catalyzing alkane oxidation by regulating oligovanadates. *Catalysis Science and Technology*, **2020**, 10, 7601-7612	5.5	3
32	Mechanical pressure-mediated Pd active sites formation in NaY zeolite catalysts for indirect oxidative carbonylation of methanol to dimethyl carbonate. *Journal of Catalysis*, **2021**, 396, 269-280	7.3	3
31	Surface Reconstruction for Forming the [IrO]-[IrO] Framework: Key Structure for Stable and Activated OER Performance in Acidic Media. *ACS Applied Materials & Interfaces*, **2021**, 13, 29654-29663	9.5	3
30	Calcination Atmosphere Regulated Morphology and Catalytic Performance of Pt/SiO2 in Gas-phase Oxidative Dehydrogenation of KA-oil. *ChemCatChem*, **2018**, 10, 5689-5697	5.2	3
29	Role of Low-Coordinated Ce in Hydride Formation and Selective Hydrogenation Reactions on CeO2 Surfaces. *ACS Catalysis*, **2022**, 12, 624-632	13.1	3
28	Identification of CO adsorption sites on MgO nanosheets by solid-state nuclear magnetic resonance spectroscopy.. *Nature Communications*, **2022**, 13, 707	17.4	2
27	A comparative study on the twinning boundaries of five-fold twinned copper and gold nanorods. *Applied Surface Science*, **2021**, 543, 148764	6.7	2
26	Wu and Gong Reply. *Physical Review Letters*, **2016**, 117, 279602	7.4	2
25	Locating structures and evolution pathways of reconstructed rutile TiO2(011) using genetic algorithm aided density functional theory calculations. *Journal of Molecular Modeling*, **2016**, 22, 114	2	2
24	Theoretical Study of Twinning Boundaries in Twinned Gold Nanorod Using Evolutionary Algorithms Aided Computational Simulations. *Journal of Physical Chemistry C*, **2019**, 123, 31103-31107	3.8	2
23	Synthesis of Lattice-Contracted Cobalt Disulfide as an Outstanding Oxygen Reduction Reaction Catalyst via Self-assembly Arrangement. *ChemSusChem*, **2021**, 14, 1388-1395	8.3	2
22	Tuning the hybridization state of Ir-O to improve the OER activity and stability of iridium pyrochlore via Zn doping. *Applied Surface Science*, **2022**, 576, 151840	6.7	1
21	CH3□Generating Capability as a Reactivity Descriptor for Metal Oxides in Oxidative Coupling of Methane. *ACS Catalysis*, **2021**, 11, 14651-14659	13.1	1
20	Light-Driven Spiral Deformation of Supramolecular Helical Microfibers by Localized Photoisomerization. *Advanced Optical Materials*,2101267	8.1	1
19	Metal substitution in the metalloporphyrin linker of metal–organic framework PCN-601 for photocatalytic CO2 reduction. *JPhys Energy*, **2021**, 3, 034016	4.9	1

18	Role of Organic Fluoride Salts in Stabilizing Niobium Oxo-Clusters Catalyzing Epoxidation. *Langmuir* , **2021**, 37, 8190-8203	4	1
17	Computational Simulation of Trapped Charge Carriers in TiO2 and Their Impacts on Photocatalytic Water Splitting. *ACS Symposium Series*, **2019**, 67-100	0.4	1
16	Modulating Photoinduced Charge Separation in Metal Azolate Frameworks. *Journal of Physical Chemistry C*, **2021**, 125, 2064-2073	3.8	1
15	[4 + 2] Cycloaddition of trifluoromethyl ketimines with 2-alkenyl azaarenes through selective C bond cleavage of CF3. *Organic Chemistry Frontiers*, **2021**, 8, 4426-4431	5.2	1
14	Two Coexisting Forms of Simple Molecules for Directing Sesqui-Unit-Cell Zeolite Nanosheets. *Chemistry of Materials*, **2021**, 33, 6934-6941	9.6	1
13	Tautomeric Dual-Site Passivation for Carbon-Based Printable Mesoscopic Perovskite Solar Cells. *Advanced Materials Interfaces*,2200326	4.6	1
12	Spontaneous Bulk-Surface Charge Separation of TiO2-{001} Nanocrystals Leads to High Activity in Photocatalytic Methane Combustion. *ACS Catalysis*,6457-6463	13.1	1
11	A first-principles molecular dynamics study on the surface lattice oxygen of ceria. *Applied Surface Science*, **2019**, 496, 143712	6.7	0
10	Strong anion exchange for improved NiCo2S4 oxygen reduction reaction via interlayer spacing manipulation. *International Journal of Hydrogen Energy*, **2022**, 47, 11224-11224	6.7	0
9	Thermodynamics Insights into the Selective Hydrogenation of Alkynes in C2 and C3 Streams. *Industrial & Engineering Chemistry Research*, **2021**, 60, 16969-16980	3.9	0
8	Relationships between the activities and Ce3+ concentrations of CeO2(111) for CO oxidation: A first-principle investigation. *Chinese Chemical Letters*, **2021**, 32, 1127-1130	8.1	0
7	In situ formation of grain boundaries on a supported hybrid to boost water oxidation activity of iridium oxide. *Nanoscale*, **2021**, 13, 13845-13857	7.7	0
6	Subtle structure matters: boosting surface-directed photoelectron transfer the introduction of specific monovalent oxygen vacancies in TiO. *Physical Chemistry Chemical Physics*, **2021**, 23, 19854-19861	3.6	0
5	Unique catalytic mechanisms of methanol dehydrogenation at Pd-doped ceria: A DFT+U study.. *Journal of Chemical Physics*, **2022**, 156, 134701	3.9	0
4	Hydrogenolysis Cleavage of the Csp2Csp3 Bond over a Metal-Free NbOPO4 Catalyst. *ACS Catalysis*,4806-4812	13.1	0
3	Photo-induced hydrophilicity at the ZnO(112 0) surface: an evolutionary algorithm-aided density functional theory study. *Physical Chemistry Chemical Physics*, **2021**, 23, 19790-19794	3.6	
2	A theoretical study of the twinned ZnO nanostructures. *Applied Surface Science*, **2022**, 571, 151295	6.7	
1	Theoretical insights into CO oxidation activities on CeO2(111) steps. *Surface Science*, **2022**, 722, 122096	1.8	