Jan Rossmeisl

List of Publications by Year in Descending Order

228 papers	43,658 citations	83 h-index	208 g-index
256 ext. papers	51,317 ext. citations	9.5 avg, IF	7.56 L-index

#	Paper	IF	Citations
228	Rationally Tailoring Catalysts for the CO Oxidation Reaction by Using DFT Calculations. *ACS Catalysis*, **2022**, 12, 116-125	13.1	1
227	Breaking with the Principles of Coreduction to Form Stoichiometric Intermetallic PdCu Nanoparticles.. *Small Methods*, **2022**, e2200420	12.8	
226	Predicting Catalytic Activity in Hydrogen Evolution Reaction. *Current Opinion in Electrochemistry*, **2022**, 101037	7.2	3
225	Free energy difference to create the M-OH intermediate of the oxygen evolution reaction by time-resolved optical spectroscopy. *Nature Materials*, **2021**,	27	5
224	Influence of the Artificial Nanostructure on the LiF Formation at the Solid Electrolyte Interphase of Carbon-Based Anodes. *ACS Applied Energy Materials*, **2021**, 4, 35-41	6.1	1
223	Three-Dimensional Carbon Electrocatalysts for CO2 or CO Reduction. *ACS Catalysis*, **2021**, 11, 533-541	13.1	14
222	A Robust PtNi Nanoframe/N-Doped Graphene Aerogel Electrocatalyst with Both High Activity and Stability. *Angewandte Chemie - International Edition*, **2021**, 60, 9590-9597	16.4	26
221	A Robust PtNi Nanoframe/N-Doped Graphene Aerogel Electrocatalyst with Both High Activity and Stability. *Angewandte Chemie*, **2021**, 133, 9676-9683	3.6	2
220	Role of Catalyst in Controlling N2 Reduction Selectivity: A Unified View of Nitrogenase and Solid Electrodes. *ACS Catalysis*, **2021**, 11, 6596-6601	13.1	11
219	Synergistic effects in oxygen evolution activity of mixed iridium-ruthenium pyrochlores. *Electrochimica Acta*, **2021**, 366, 137327	6.7	5
218	Pt-Sn-Co nanocubes as highly active catalysts for ethanol electro-oxidation. *Journal of Catalysis*, **2021**, 393, 247-258	7.3	7
217	Highly active, selective, and stable Pd single-atom catalyst anchored on N-doped hollow carbon sphere for electrochemical H2O2 synthesis under acidic conditions. *Journal of Catalysis*, **2021**, 393, 313-323	7.3	10
216	Surface electrocatalysis on high-entropy alloys. *Current Opinion in Electrochemistry*, **2021**, 26, 100651	7.2	18
215	Self-supported Pt-CoO networks combining high specific activity with high surface area for oxygen reduction. *Nature Materials*, **2021**, 20, 208-213	27	54
214	Lifting the discrepancy between experimental results and the theoretical predictions for the catalytic activity of RuO(110) towards oxygen evolution reaction. *Physical Chemistry Chemical Physics*, **2021**, 23, 19141-19145	3.6	2
213	Engendering Unprecedented Activation of Oxygen Evolution via Rational Pinning of Ni Oxidation State in Prototypical Perovskite: Close Juxtaposition of Synthetic Approach and Theoretical Conception. *ACS Catalysis*, **2021**, 11, 985-997	13.1	2
212	pH and Anion Effects on Cu Phosphate Interfaces for CO Electroreduction. *ACS Catalysis*, **2021**, 11, 1128-1135	13.1	7

211	Chemisorbed oxygen or surface oxides steer the selectivity in Pd electrocatalytic propene oxidation observed by operando Pd L-edge X-ray absorption spectroscopy. *Catalysis Science and Technology*, **2021**, 11, 3347-3352	5.5	1
210	Complex-Solid-Solution Electrocatalyst Discovery by Computational Prediction and High-Throughput Experimentation*. *Angewandte Chemie - International Edition*, **2021**, 60, 6932-6937	16.4	28
209	Complex-Solid-Solution Electrocatalyst Discovery by Computational Prediction and High-Throughput Experimentation**. *Angewandte Chemie*, **2021**, 133, 7008-7013	3.6	4
208	Morphology and mechanism of highly selective Cu(II) oxide nanosheet catalysts for carbon dioxide electroreduction. *Nature Communications*, **2021**, 12, 794	17.4	45
207	What Atomic Positions Determines Reactivity of a Surface? Long-Range, Directional Ligand Effects in Metallic Alloys. *Advanced Science*, **2021**, 8, 2003357	13.6	9
206	What Makes High-Entropy Alloys Exceptional Electrocatalysts?. *Angewandte Chemie - International Edition*, **2021**,	16.4	19
205	Electrochemical Nitric Oxide Reduction on Metal Surfaces. *Angewandte Chemie - International Edition*, **2021**, 60, 21966-21972	16.4	23
204	Electrochemical Nitric Oxide Reduction on Metal Surfaces. *Angewandte Chemie*, **2021**, 133, 22137-22143	3.6	5
203	Bayesian Optimization of High-Entropy Alloy Compositions for Electrocatalytic Oxygen Reduction*. *Angewandte Chemie - International Edition*, **2021**, 60, 24144-24152	16.4	16
202	The role of an interface in stabilizing reaction intermediates for hydrogen evolution in aprotic electrolytes. *Chemical Science*, **2020**, 11, 3914-3922	9.4	12
201	Oxygen evolution reaction: a perspective on a decade of atomic scale simulations. *Chemical Science*, **2020**, 11, 2943-2950	9.4	34
200	Insights in the Oxygen Reduction Reaction: From Metallic Electrocatalysts to Diporphyrins. *ACS Catalysis*, **2020**, 10, 5979-5989	13.1	27
199	Fundamental Atomic Insight in Electrocatalysis **2020**, 1473-1503		1
198	High-Entropy Alloys as Catalysts for the CO2 and CO Reduction Reactions. *ACS Catalysis*, **2020**, 10, 2169-2176	13.1	108
197	Electrochemical Interface during Corrosion of Copper in Anoxic Sulfide-Containing Groundwater: A Computational Study. *Journal of Physical Chemistry C*, **2020**, 124, 469-481	3.8	6
196	Uncovering the electrochemical interface of low-index copper surfaces in deep groundwater environments. *Electrochimica Acta*, **2020**, 362, 137111	6.7	3
195	P-block single-metal-site tin/nitrogen-doped carbon fuel cell cathode catalyst for oxygen reduction reaction. *Nature Materials*, **2020**, 19, 1215-1223	27	127
194	Realistic Cyclic Voltammograms from Ab Initio Simulations in Alkaline and Acidic Electrolytes. *Journal of Physical Chemistry C*, **2020**, 124, 20055-20065	3.8	16

193	Mechanistic reaction pathways of enhanced ethylene yields during electroreduction of CO-CO co-feeds on Cu and Cu-tandem electrocatalysts. *Nature Nanotechnology*, **2019**, 14, 1063-1070	28.7	130
192	Multiple Reaction Paths for CO Oxidation on a 2D SnOx Nano-Oxide on the Pt(110) Surface: Intrinsic Reactivity and Spillover. *Advanced Materials Interfaces*, **2019**, 6, 1801874	4.6	4
191	Efficient CO2 to CO electrolysis on solid Ni-N-C catalysts at industrial current densities. *Energy and Environmental Science*, **2019**, 12, 640-647	35.4	228
190	Unraveling Mechanistic Reaction Pathways of the Electrochemical CO2 Reduction on Fe-N-C Single-Site Catalysts. *ACS Energy Letters*, **2019**, 4, 1663-1671	20.1	91
189	Electrochemical Synthesis of High-Value Chemicals: Detection of Key Reaction Intermediates and Products Combining Gas Chromatography-Mass Spectrometry and in Situ Infrared Spectroscopy. *Journal of Physical Chemistry C*, **2019**,	3.8	2
188	Ab Initio Cyclic Voltammetry on Cu(111), Cu(100) and Cu(110) in Acidic, Neutral and Alkaline Solutions. *ChemPhysChem*, **2019**, 20, 3096-3105	3.2	36
187	Activity-Selectivity Trends in the Electrochemical Production of Hydrogen Peroxide over Single-Site Metal-Nitrogen-Carbon Catalysts. *Journal of the American Chemical Society*, **2019**, 141, 12372-12381	16.4	236
186	Electrochemical CO2 Reduction: Classifying Cu Facets. *ACS Catalysis*, **2019**, 9, 7894-7899	13.1	89
185	Electrochemical Reduction of CO2 on Metal-Nitrogen-Doped Carbon Catalysts. *ACS Catalysis*, **2019**, 9, 7270-7284	13.1	158
184	Ligand-Dependent Energetics for Dehydrogenation: Implications in Li-Ion Battery Electrolyte Stability and Selective Oxidation Catalysis of Hydrogen-Containing Molecules. *Chemistry of Materials*, **2019**, 31, 5464-5474	9.6	16
183	Trace anodic migration of iridium and titanium ions and subsequent cathodic selectivity degradation in acid electrolysis systems. *Materials Today Energy*, **2019**, 14, 100352	7	3
182	Enhanced Oxygen Reduction Reaction on Fe/N/C Catalyst in Acetate Buffer Electrolyte. *ACS Catalysis*, **2019**, 9, 3082-3089	13.1	23
181	Towards an atomistic understanding of electrocatalytic partial hydrocarbon oxidation: propene on palladium. *Energy and Environmental Science*, **2019**, 12, 1055-1067	35.4	20
180	Catalyst design criteria and fundamental limitations in the electrochemical synthesis of dimethyl carbonate. *Green Chemistry*, **2019**, 21, 6200-6209	10	5
179	Electrochemical CO Reduction: A Property of the Electrochemical Interface. *Journal of the American Chemical Society*, **2019**, 141, 1506-1514	16.4	76
178	High-Entropy Alloys as a Discovery Platform for Electrocatalysis. *Joule*, **2019**, 3, 834-845	27.8	202
177	Climbing the 3D Volcano for the Oxygen Reduction Reaction Using Porphyrin Motifs. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 611-617	8.3	24
176	Electrochemically Generated Copper Carbonyl for Selective Dimethyl Carbonate Synthesis. *ACS Catalysis*, **2019**, 9, 859-866	13.1	12

175	Frontispiece: Elucidation of the Oxygen Reduction Volcano in Alkaline Media using a Copper–Platinum(111) Alloy. *Angewandte Chemie - International Edition*, **2018**, 57,	16.4	1
174	pH Effects on the Selectivity of the Electrocatalytic CO2 Reduction on Graphene-Embedded Fe–N–C Motifs: Bridging Concepts between Molecular Homogeneous and Solid-State Heterogeneous Catalysis. *ACS Energy Letters*, **2018**, 3, 812-817	20.1	104
173	Fundamental limitation of electrocatalytic methane conversion to methanol. *Physical Chemistry Chemical Physics*, **2018**, 20, 11152-11159	3.6	47
172	Electrocatalytic transformation of HF impurity to H2 and LiF in lithium-ion batteries. *Nature Catalysis*, **2018**, 1, 255-262	36.5	83
171	Elucidation of the Oxygen Reduction Volcano in Alkaline Media using a Copper-Platinum(111) Alloy. *Angewandte Chemie - International Edition*, **2018**, 57, 2800-2805	16.4	56
170	Elucidation of the Oxygen Reduction Volcano in Alkaline Media using a Copper–Platinum(111) Alloy. *Angewandte Chemie*, **2018**, 130, 2850-2855	3.6	5
169	Modeling the adsorption of sulfur containing molecules and their hydrodesulfurization intermediates on the Co-promoted MoS2 catalyst by DFT. *Journal of Catalysis*, **2018**, 358, 131-140	7.3	34
168	Oxidation of Ethylene Carbonate on Li Metal Oxide Surfaces. *Journal of Physical Chemistry C*, **2018**, 122, 10442-10449	3.8	41
167	Toward the Decentralized Electrochemical Production of H2O2: A Focus on the Catalysis. *ACS Catalysis*, **2018**, 8, 4064-4081	13.1	341
166	On the thickness of the double layer in ionic liquids. *Physical Chemistry Chemical Physics*, **2018**, 20, 10275-10285	3.6	27
165	Importance of Surface IrO in Stabilizing RuO for Oxygen Evolution. *Journal of Physical Chemistry B*, **2018**, 122, 947-955	3.4	58
164	Trends in Activity and Dissolution on RuO2 under Oxygen Evolution Conditions: Particles versus Well-Defined Extended Surfaces. *ACS Energy Letters*, **2018**, 3, 2045-2051	20.1	77
163	CO2 electroreduction on copper-cobalt nanoparticles: Size and composition effect. *Nano Energy*, **2018**, 53, 27-36	17.1	64
162	Fundamental Atomic Insight in Electrocatalysis **2018**, 1-31		4
161	Operando XAS Study of the Surface Oxidation State on a Monolayer IrO on RuO and Ru Oxide Based Nanoparticles for Oxygen Evolution in Acidic Media. *Journal of Physical Chemistry B*, **2018**, 122, 878-887	3.4	45
160	The Influence of Inert Ions on the Reactivity of Manganese Oxides. *Journal of Physical Chemistry C*, **2018**, 122, 216-226	3.8	9
159	Rationality in the new oxygen evolution catalyst development. *Current Opinion in Electrochemistry*, **2018**, 12, 218-224	7.2	18
158	Topotactic Growth of Edge-Terminated MoS from MoO Nanocrystals. *ACS Nano*, **2018**, 12, 5351-5358	16.7	18

157	Active-Phase Formation and Stability of Gd/Pt(111) Electrocatalysts for Oxygen Reduction: An In Situ Grazing Incidence X-Ray Diffraction Study. *Chemistry - A European Journal*, **2018**, 24, 12280-12290	4.8	10
156	Synergetic Surface Sensitivity of Photoelectrochemical Water Oxidation on TiO2 (Anatase) Electrodes. *Journal of Physical Chemistry C*, **2017**, 121, 6024-6032	3.8	13
155	Single site porphyrine-like structures advantages over metals for selective electrochemical CO2 reduction. *Catalysis Today*, **2017**, 288, 74-78	5.3	79
154	Orientation-Dependent Oxygen Evolution on RuO2 without Lattice Exchange. *ACS Energy Letters*, **2017**, 2, 876-881	20.1	165
153	Modeling the active sites of Co-promoted MoS particles by DFT. *Physical Chemistry Chemical Physics* , **2017**, 19, 2017-2024	3.6	22
152	Accessing the Inaccessible: Analyzing the Oxygen Reduction Reaction in the Diffusion Limit. *ACS Applied Materials & Interfaces*, **2017**, 9, 38176-38180	9.5	15
151	Understanding activity and selectivity of metal-nitrogen-doped carbon catalysts for electrochemical reduction of CO. *Nature Communications*, **2017**, 8, 944	17.4	604
150	Electrochemical CO Reduction: A Classification Problem. *ChemPhysChem*, **2017**, 18, 3266-3273	3.2	271
149	Enhanced Carbon Dioxide Electroreduction to Carbon Monoxide over Defect-Rich Plasma-Activated Silver Catalysts. *Angewandte Chemie*, **2017**, 129, 11552-11556	3.6	42
148	Enhanced Carbon Dioxide Electroreduction to Carbon Monoxide over Defect-Rich Plasma-Activated Silver Catalysts. *Angewandte Chemie - International Edition*, **2017**, 56, 11394-11398	16.4	136
147	Role of the Band Gap for the Interaction Energy of Coadsorbed Fragments. *Journal of Physical Chemistry C*, **2017**, 121, 18608-18614	3.8	12
146	Modelling pH and potential in dynamic structures of the water/Pt(111) interface on the atomic scale. *Physical Chemistry Chemical Physics*, **2017**, 19, 23505-23514	3.6	40
145	Towards identifying the active sites on RuO2(110) in catalyzing oxygen evolution. *Energy and Environmental Science*, **2017**, 10, 2626-2637	35.4	185
144	Defect Chemistry and Electrical Conductivity of Sm-Doped La1−xSrxCoO3−δ for Solid Oxide Fuel Cells. *Journal of Physical Chemistry C*, **2017**, 121, 15017-15027	3.8	10
143	A DFT Structural Investigation of New Bimetallic PtSnx Surface Alloys Formed on the Pt(110) Surface and Their Interaction with Carbon Monoxide. *Journal of Physical Chemistry C*, **2016**, 120, 25306-25316	3.8	4
142	Investigating the coverage dependent behaviour of CO on Gd/Pt(111). *Physical Chemistry Chemical Physics*, **2016**, 18, 29732-29739	3.6	4
141	Probing the nanoscale structure of the catalytically active overlayer on Pt alloys with rare earths. *Nano Energy*, **2016**, 29, 249-260	17.1	40
140	Finite Bias Calculations to Model Interface Dipoles in Electrochemical Cells at the Atomic Scale. *Journal of Physical Chemistry C*, **2016**, 120, 13485-13491	3.8	29

139	Targeted design of □MnO2 based catalysts for oxygen reduction. *Electrochimica Acta*, **2016**, 191, 452-461	6.7	23
138	On the pH dependence of electrochemical proton transfer barriers. *Catalysis Today*, **2016**, 262, 36-40	5.3	68
137	Correlation between diffusion barriers and alloying energy in binary alloys. *Physical Chemistry Chemical Physics*, **2016**, 18, 3302-7	3.6	24
136	Oxygen Reduction Reaction on Pt Overlayers Deposited onto a Gold Film: Ligand, Strain, and Ensemble Effect. *ACS Catalysis*, **2016**, 6, 671-676	13.1	66
135	Toward sustainable fuel cells. *Science*, **2016**, 354, 1378-1379	33.3	281
134	pH in Grand Canonical Statistics of an Electrochemical Interface. *Journal of Physical Chemistry C*, **2016**, 120, 29135-29143	3.8	60
133	Tuning the activity of Pt alloy electrocatalysts by means of the lanthanide contraction. *Science*, **2016**, 352, 73-6	33.3	575
132	Water at Interfaces. *Chemical Reviews*, **2016**, 116, 7698-726	68.1	388
131	Atomic-Scale Analysis of the RuO2/Water Interface under Electrochemical Conditions. *Journal of Physical Chemistry C*, **2016**, 120, 8096-8103	3.8	35
130	Beyond the top of the volcano? □A unified approach to electrocatalytic oxygen reduction and oxygen evolution. *Nano Energy*, **2016**, 29, 126-135	17.1	195
129	Relation between Hydrogen Evolution and Hydrodesulfurization Catalysis. *ChemCatChem*, **2016**, 8, 3334-3337	5.2	15
128	Atomic scale analysis of sterical effects in the adsorption of 4,6-dimethyldibenzothiophene on a CoMoS hydrotreating catalyst. *Journal of Catalysis*, **2016**, 344, 121-128	7.3	42
127	Ketene as a Reaction Intermediate in the Carbonylation of Dimethyl Ether to Methyl Acetate over Mordenite. *Angewandte Chemie - International Edition*, **2015**, 54, 7261-4	16.4	64
126	First principles investigation of the activity of thin film Pt, Pd and Au surface alloys for oxygen reduction. *Physical Chemistry Chemical Physics*, **2015**, 17, 11647-57	3.6	35
125	Widely available active sites on Ni2P for electrochemical hydrogen evolution--insights from first principles calculations. *Physical Chemistry Chemical Physics*, **2015**, 17, 10823-9	3.6	100
124	Comparison between the Oxygen Reduction Reaction Activity of Pd5Ce and Pt5Ce: The Importance of Crystal Structure. *ACS Catalysis*, **2015**, 5, 6032-6040	13.1	18
123	Oxygen reduction on nanocrystalline ruthenia □local structure effects. *RSC Advances*, **2015**, 5, 1235-1243	3.7	17
122	Towards first principles modeling of electrochemical electrode□electrolyte interfaces. *Surface Science*, **2015**, 631, 2-7	1.8	72

121	Enhancing Activity for the Oxygen Evolution Reaction: The Beneficial Interaction of Gold with Manganese and Cobalt Oxides. *ChemCatChem*, **2015**, 7, 149-154	5.2	99
120	Toward an Active and Stable Catalyst for Oxygen Evolution in Acidic Media: Ti-Stabilized MnO2. *Advanced Energy Materials*, **2015**, 5, 1500991	21.8	131
119	Ketene as a Reaction Intermediate in the Carbonylation of Dimethyl Ether to Methyl Acetate over Mordenite. *Angewandte Chemie*, **2015**, 127, 7369-7372	3.6	6
118	Mechanistic Pathway in the Electrochemical Reduction of CO2 on RuO2. *ACS Catalysis*, **2015**, 5, 4075-4081	13.1	95
117	A Linear Response DFT+U Study of Trends in the Oxygen Evolution Activity of Transition Metal Rutile Dioxides. *Journal of Physical Chemistry C*, **2015**, 119, 4827-4833	3.8	72
116	The Influence of Particle Shape and Size on the Activity of Platinum Nanoparticles for Oxygen Reduction Reaction: A Density Functional Theory Study. *Catalysis Letters*, **2014**, 144, 380-388	2.8	57
115	Thermochemistry and micro-kinetic analysis of methanol synthesis on ZnO (0 0 0 1). *Journal of Catalysis*, **2014**, 309, 397-407	7.3	46
114	Elucidating the activity of stepped Pt single crystals for oxygen reduction. *Physical Chemistry Chemical Physics*, **2014**, 16, 13625-9	3.6	79
113	H(2) production through electro-oxidation of SO(2): identifying the fundamental limitations. *Physical Chemistry Chemical Physics*, **2014**, 16, 9572-9	3.6	27
112	Pt Skin Versus Pt Skeleton Structures of Pt3Sc as Electrocatalysts for Oxygen Reduction. *Topics in Catalysis*, **2014**, 57, 245-254	2.3	36
111	Beyond the volcano limitations in electrocatalysis--oxygen evolution reaction. *Physical Chemistry Chemical Physics*, **2014**, 16, 13682-8	3.6	239
110	Ab Initio Thermodynamic Modeling of Electrified Metal□Oxide Interfaces: Consistent Treatment of Electronic and Ionic Chemical Potentials. *Journal of Physical Chemistry C*, **2014**, 118, 22663-22671	3.8	11
109	Trends in the electrochemical synthesis of H2O2: enhancing activity and selectivity by electrocatalytic site engineering. *Nano Letters*, **2014**, 14, 1603-8	11.5	352
108	Intermetallic Alloys as CO Electroreduction Catalysts□Role of Isolated Active Sites. *ACS Catalysis*, **2014**, 4, 2268-2273	13.1	76
107	Platinum redispersion on metal oxides in low temperature fuel cells. *Physical Chemistry Chemical Physics*, **2013**, 15, 3279-85	3.6	10
106	Ni□Fe□S Cubanes in CO2 Reduction Electrocatalysis: A DFT Study. *ACS Catalysis*, **2013**, 3, 2640-2643	13.1	53
105	Enabling direct H2O2 production through rational electrocatalyst design. *Nature Materials*, **2013**, 12, 1137-43	27	649
104	Origin of electrolyte-dopant dependent sulfur poisoning of SOFC anodes. *Physical Chemistry Chemical Physics*, **2013**, 15, 6769-72	3.6	15

103	Generalized trends in the formation energies of perovskite oxides. *Physical Chemistry Chemical Physics*, **2013**, 15, 7526-33	3.6	67
102	Modeling of the symmetry factor of electrochemical proton discharge via the Volmer reaction. *Catalysis Today*, **2013**, 202, 168-174	5.3	15
101	Number of outer electrons as descriptor for adsorption processes on transition metals and their oxides. *Chemical Science*, **2013**, 4, 1245	9.4	211
100	Avoiding pitfalls in the modeling of electrochemical interfaces. *Chemical Physics Letters*, **2013**, 555, 145-148	2.3	47
99	Electrochemical CO2 and CO Reduction on Metal-Functionalized Porphyrin-like Graphene. *Journal of Physical Chemistry C*, **2013**, 117, 9187-9195	3.8	218
98	Tandem cathode for proton exchange membrane fuel cells. *Physical Chemistry Chemical Physics*, **2013**, 15, 9326-34	3.6	34
97	First principles investigation of zinc-anode dissolution in zinc-air batteries. *Physical Chemistry Chemical Physics*, **2013**, 15, 6416-21	3.6	31
96	pH in atomic scale simulations of electrochemical interfaces. *Physical Chemistry Chemical Physics*, **2013**, 15, 10321-5	3.6	100
95	DFT based study of transition metal nano-clusters for electrochemical NH3 production. *Physical Chemistry Chemical Physics*, **2013**, 15, 7785-95	3.6	116
94	Activity and Selectivity for O2 Reduction to H2O2 on Transition Metal Surfaces. *ECS Transactions*, **2013**, 58, 53-62	1	9
93	Oxidative trends of TiO2 hole trapping at anatase and rutile surfaces. *Energy and Environmental Science*, **2012**, 5, 9866	35.4	37
92	Design of an Active Site towards Optimal Electrocatalysis: Overlayers, Surface Alloys and Near-Surface Alloys of Cu/Pt(111). *Angewandte Chemie*, **2012**, 124, 12015-12018	3.6	13
91	Design of an active site towards optimal electrocatalysis: overlayers, surface alloys and near-surface alloys of Cu/Pt(111). *Angewandte Chemie - International Edition*, **2012**, 51, 11845-8	16.4	89
90	Unifying the 2e(-) and 4e(-) Reduction of Oxygen on Metal Surfaces. *Journal of Physical Chemistry Letters*, **2012**, 3, 2948-51	6.4	206
89	Physical and chemical nature of the scaling relations between adsorption energies of atoms on metal surfaces. *Physical Review Letters*, **2012**, 108, 116103	7.4	186
88	Identifying active surface phases for metal oxide electrocatalysts: a study of manganese oxide bi-functional catalysts for oxygen reduction and water oxidation catalysis. *Physical Chemistry Chemical Physics*, **2012**, 14, 14010-22	3.6	270
87	Electrochemical Hydrogen Evolution: Sabatier's Principle and the Volcano Plot. *Journal of Chemical Education*, **2012**, 89, 1595-1599	2.4	155
86	Pt5Gd as a highly active and stable catalyst for oxygen electroreduction. *Journal of the American Chemical Society*, **2012**, 134, 16476-9	16.4	185

85	Simulating Linear Sweep Voltammetry from First-Principles: Application to Electrochemical Oxidation of Water on Pt(111) and Pt3Ni(111). *Journal of Physical Chemistry C*, **2012**, 116, 4698-4704	3.8	64
84	Bifunctional anode catalysts for direct methanol fuel cells. *Energy and Environmental Science*, **2012**, 5, 8335	35.4	138
83	A theoretical evaluation of possible transition metal electro-catalysts for N2 reduction. *Physical Chemistry Chemical Physics*, **2012**, 14, 1235-45	3.6	810
82	Methanol Oxidation on Model Elemental and Bimetallic Transition Metal Surfaces. *Journal of Physical Chemistry C*, **2012**, 116, 11980-11986	3.8	72
81	Understanding the electrocatalysis of oxygen reduction on platinum and its alloys. *Energy and Environmental Science*, **2012**, 5, 6744	35.4	852
80	Photoelectrocatalysis and electrocatalysis on silicon electrodes decorated with cubane-like clusters. *Journal of Photonics for Energy*, **2012**, 2, 026001	1.2	16
79	Metal Oxide-Supported Platinum Overlayers as Proton-Exchange Membrane Fuel Cell Cathodes. *ChemCatChem*, **2012**, 4, 228-235	5.2	42
78	Volcano Relations for Oxidation of Hydrogen Halides over Rutile Oxide Surfaces. *ChemCatChem*, **2012**, 4, 1856-1861	5.2	11
77	Solar hydrogen production with semiconductor metal oxides: new directions in experiment and theory. *Physical Chemistry Chemical Physics*, **2012**, 14, 49-70	3.6	171
76	Universality in Oxygen Reduction Electrocatalysis on Metal Surfaces. *ACS Catalysis*, **2012**, 2, 1654-1660	13.1	360
75	The atomic structure of protons and hydrides in Sm1.92Ca0.08Sn2O7□ pyrochlore from DFT calculations and FTIR spectroscopy. *Journal of Applied Physics*, **2012**, 112, 033705	2.5	2
74	Electronic hole transfer in rutile and anatase TiO2: Effect of a delocalization error in the density functional theory on the charge transfer barrier height. *Physical Review B*, **2011**, 84,	3.3	13
73	Tuning the activity of Pt(111) for oxygen electroreduction by subsurface alloying. *Journal of the American Chemical Society*, **2011**, 133, 5485-91	16.4	385
72	Hydrogen evolution on Au(111) covered with submonolayers of Pd. *Physical Review B*, **2011**, 84,	3.3	43
71	Prediction of solid oxide fuel cell cathode activity with first-principles descriptors. *Energy and Environmental Science*, **2011**, 4, 3966	35.4	345
70	Universal transition state scaling relations for (de)hydrogenation over transition metals. *Physical Chemistry Chemical Physics*, **2011**, 13, 20760-5	3.6	295
69	Bioinspired molecular co-catalysts bonded to a silicon photocathode for solar hydrogen evolution. *Nature Materials*, **2011**, 10, 434-8	27	556
68	Trends in oxygen reduction and methanol activation on transition metal chalcogenides. *Electrochimica Acta*, **2011**, 56, 9783-9788	6.7	48

67	The Pt(111)/electrolyte interface under oxygen reduction reaction conditions: an electrochemical impedance spectroscopy study. *Langmuir*, **2011**, 27, 2058-66	4	157
66	Trends in Metal Oxide Stability for Nanorods, Nanotubes, and Surfaces. *Journal of Physical Chemistry C*, **2011**, 115, 2244-2252	3.8	46
65	Universality in Oxygen Evolution Electrocatalysis on Oxide Surfaces. *ChemCatChem*, **2011**, 3, 1159-1165	5.2	2321
64	Tailoring the Activity for Oxygen Evolution Electrocatalysis on Rutile TiO2(110) by Transition-Metal Substitution. *ChemCatChem*, **2011**, 3, 1607-1611	5.2	146
63	Atomic-Scale Modeling of Particle Size Effects for the Oxygen Reduction Reaction on Pt. *Catalysis Letters*, **2011**, 141, 909-913	2.8	193
62	Density functional studies of functionalized graphitic materials with late transition metals for Oxygen Reduction Reactions. *Physical Chemistry Chemical Physics*, **2011**, 13, 15639-43	3.6	342
61	The Sabatier Principle Illustrated by Catalytic H2O2 Decomposition on Metal Surfaces. *Journal of Chemical Education*, **2011**, 88, 1711-1715	2.4	33
60	Thermodynamic and kinetic properties of hydrogen defect pairs in SrTiO3 from density functional theory. *Physical Chemistry Chemical Physics*, **2011**, 13, 15256-63	3.6	15
59	On the behavior of Brønsted-Evans-Polanyi relations for transition metal oxides. *Journal of Chemical Physics*, **2011**, 134, 244509	3.9	108
58	Electronic hole localization in rutile and anatase TiO2 □Self-interaction correction in □SCF DFT. *Chemical Physics Letters*, **2011**, 506, 42-45	2.5	28
57	Standard hydrogen electrode and potential of zero charge in density functional calculations. *Physical Review B*, **2011**, 84,	3.3	100
56	Ab initio charge analysis of pure and hydrogenated perovskites. *Journal of Applied Physics*, **2011**, 109, 033702	2.5	15
55	Bio-inspired co-catalysts bonded to a silicon photocathode for solar hydrogen evolution **2011**,		1
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