Manos Mavrikakis

List of Publications by Citations

281 papers	30,512 citations	76 h-index	171 g-index
305 ext. papers	33,559 ext. citations	9.4 avg, IF	7.42 L-index

#	Paper	IF	Citations
281	Highly crystalline multimetallic nanoframes with three-dimensional electrocatalytic surfaces. *Science*, **2014**, 343, 1339-43	33.3	1989
280	Effect of Strain on the Reactivity of Metal Surfaces. *Physical Review Letters*, **1998**, 81, 2819-2822	7.4	1680
279	Ru-Pt core-shell nanoparticles for preferential oxidation of carbon monoxide in hydrogen. *Nature Materials*, **2008**, 7, 333-8	27	1057
278	On the origin of the catalytic activity of gold nanoparticles for low-temperature CO oxidation. *Journal of Catalysis*, **2004**, 223, 232-235	7.3	1017
277	Universality in Heterogeneous Catalysis. *Journal of Catalysis*, **2002**, 209, 275-278	7.3	1007
276	Controlling the catalytic activity of platinum-monolayer electrocatalysts for oxygen reduction with different substrates. *Angewandte Chemie - International Edition*, **2005**, 44, 2132-5	16.4	948
275	Alloy catalysts designed from first principles. *Nature Materials*, **2004**, 3, 810-5	27	917
274	Mechanism of Methanol Synthesis on Cu through CO2 and CO Hydrogenation. *ACS Catalysis*, **2011**, 1, 365-384	13.1	801
273	Electronic structure and catalysis on metal surfaces. *Annual Review of Physical Chemistry*, **2002**, 53, 319-48	15.7	801
272	Platinum Monolayer Fuel Cell Electrocatalysts. *Topics in Catalysis*, **2007**, 46, 249-262	2.3	752
271	NANOCATALYSTS. Platinum-based nanocages with subnanometer-thick walls and well-defined, controllable facets. *Science*, **2015**, 349, 412-6	33.3	724
270	On the mechanism of low-temperature water gas shift reaction on copper. *Journal of the American Chemical Society*, **2008**, 130, 1402-14	16.4	707
269	Making gold less noble. *Catalysis Letters*, **2000**, 64, 101-106	2.8	569
268	Adsorption and dissociation of O2 on Pt-Co and Pt-Fe alloys. *Journal of the American Chemical Society*, **2004**, 126, 4717-25	16.4	559
267	Alkali-stabilized Pt-OHx species catalyze low-temperature water-gas shift reactions. *Science*, **2010**, 329, 1633-6	33.3	535
266	Mixed-metal pt monolayer electrocatalysts for enhanced oxygen reduction kinetics. *Journal of the American Chemical Society*, **2005**, 127, 12480-1	16.4	510
265	Catalytically active Au-O(OH)x-species stabilized by alkali ions on zeolites and mesoporous oxides. *Science*, **2014**, 346, 1498-501	33.3	437

264	CO activation pathways and the mechanism of Fischer Tropsch synthesis. *Journal of Catalysis*, **2010**, 272, 287-297	7.3	414
263	Mechanism of the Water Gas Shift Reaction on Pt: First Principles, Experiments, and Microkinetic Modeling. *Journal of Physical Chemistry C*, **2008**, 112, 4608-4617	3.8	392
262	Atomic layer-by-layer deposition of Pt on Pd nanocubes for catalysts with enhanced activity and durability toward oxygen reduction. *Nano Letters*, **2014**, 14, 3570-6	11.5	380
261	Palladium-platinum core-shell icosahedra with substantially enhanced activity and durability towards oxygen reduction. *Nature Communications*, **2015**, 6, 7594	17.4	365
260	Competitive paths for methanol decomposition on Pt(111). *Journal of the American Chemical Society*, **2004**, 126, 3910-9	16.4	360
259	Hydrogen adsorption, absorption and diffusion on and in transition metal surfaces: A DFT study. *Surface Science*, **2012**, 606, 679-689	1.8	312
258	Surface and subsurface hydrogen: adsorption properties on transition metals and near-surface alloys. *Journal of Physical Chemistry B*, **2005**, 109, 3460-71	3.4	308
257	Oxygenate reaction pathways on transition metal surfaces. *Journal of Molecular Catalysis A*, **1998**, 131, 135-147		306
256	Adsorption and Dissociation of O2on Gold Surfaces: Effect of Steps and Strain. *Journal of Physical Chemistry B*, **2003**, 107, 9298-9307	3.4	296
255	A first-principles study of methanol decomposition on Pt(111). *Journal of the American Chemical Society*, **2002**, 124, 7193-201	16.4	296
254	DFT studies for cleavage of C?C and C?O bonds in surface species derived from ethanol on Pt(111). *Journal of Catalysis*, **2003**, 218, 178-190	7.3	260
253	Modeling ethanol decomposition on transition metals: a combined application of scaling and Br sted-Evans-Polanyi relations. *Journal of the American Chemical Society*, **2009**, 131, 5809-15	16.4	245
252	Preferential CO oxidation in hydrogen: reactivity of core-shell nanoparticles. *Journal of the American Chemical Society*, **2010**, 132, 7418-28	16.4	239
251	Atomic and molecular adsorption on Pt(111). *Surface Science*, **2005**, 587, 159-174	1.8	230
250	Why Au and Cu Are More Selective Than Pt for Preferential Oxidation of CO at Low Temperature. *Catalysis Letters*, **2004**, 93, 93-100	2.8	214
249	Platinum monolayer electrocatalysts for oxygen reduction. *Electrochimica Acta*, **2007**, 52, 2257-2263	6.7	209
248	A Cu/Pt near-surface alloy for water-gas shift catalysis. *Journal of the American Chemical Society*, **2007**, 129, 6485-90	16.4	209
247	Improving electrocatalysts for O(2) reduction by fine-tuning the Pt-support interaction: Pt monolayer on the surfaces of a Pd(3)Fe(111) single-crystal alloy. *Journal of the American Chemical Society*, **2009**, 131, 12755-62	16.4	202

246	Water-mediated proton hopping on an iron oxide surface. *Science*, **2012**, 336, 889-93	33.3	199
245	Trends in low-temperature water gas shift reactivity on transition metals. *Journal of Catalysis*, **2005**, 229, 265-275	7.3	194
244	Bimetallic and Ternary Alloys for Improved Oxygen Reduction Catalysis. *Topics in Catalysis*, **2007**, 46, 276-284	2.3	188
243	Molecular-level descriptions of surface chemistry in kinetic models using density functional theory. *Chemical Engineering Science*, **2004**, 59, 4679-4691	4.4	188
242	Atomic and molecular adsorption on Rh(111). *Journal of Chemical Physics*, **2002**, 117, 6737-6744	3.9	187
241	Improved oxygen reduction reactivity of platinum monolayers on transition metal surfaces. *Surface Science*, **2008**, 602, L89-L94	1.8	184
240	Atomic layer-by-layer deposition of platinum on palladium octahedra for enhanced catalysts toward the oxygen reduction reaction. *ACS Nano*, **2015**, 9, 2635-47	16.7	180
239	Methanol Decomposition on Cu(111): A DFT Study. *Journal of Catalysis*, **2002**, 208, 291-300	7.3	168
238	Structure sensitivity of methanol electrooxidation on transition metals. *Journal of the American Chemical Society*, **2009**, 131, 14381-9	16.4	165
237	Partial and complete reduction of O2 by hydrogen on transition metal surfaces. *Surface Science*, **2010**, 604, 1565-1575	1.8	164
236	A first-principles study of surface and subsurface H on and in Ni(111): diffusional properties and coverage-dependent behavior. *Surface Science*, **2003**, 540, 215-229	1.8	160
235	Trends in Formic Acid Decomposition on Model Transition Metal Surfaces: A Density Functional Theory study. *ACS Catalysis*, **2014**, 4, 4434-4445	13.1	159
234	Adsorption and dissociation of O2 on Cu(): thermochemistry, reaction barrier and the effect of strain. *Surface Science*, **2001**, 494, 131-144	1.8	154
233	Reactivity descriptors for direct methanol fuel cell anode catalysts. *Surface Science*, **2008**, 602, 3424-3431	1.8	150
232	Controlling the Catalytic Activity of Platinum-Monolayer Electrocatalysts for Oxygen Reduction with Different Substrates. *Angewandte Chemie*, **2005**, 117, 2170-2173	3.6	150
231	Stabilization of copper catalysts for liquid-phase reactions by atomic layer deposition. *Angewandte Chemie - International Edition*, **2013**, 52, 13808-12	16.4	146
230	Bifunctional anode catalysts for direct methanol fuel cells. *Energy and Environmental Science*, **2012**, 5, 8335	35.4	138
229	Structure Sensitivity of CO Dissociation on Rh Surfaces. *Catalysis Letters*, **2002**, 81, 153-156	2.8	135

228	Effect of subsurface oxygen on the reactivity of the Ag(111) surface. *Journal of the American Chemical Society*, **2005**, 127, 12823-7	16.4	133
227	Atomic and Molecular Adsorption on Ir(111). *Journal of Physical Chemistry B*, **2004**, 108, 987-994	3.4	132
226	Synthesis and Characterization of Pt-Ag Alloy Nanocages with Enhanced Activity and Durability toward Oxygen Reduction. *Nano Letters*, **2016**, 16, 6644-6649	11.5	132
225	Near-surface alloys for hydrogen fuel cell applications. *Catalysis Today*, **2006**, 111, 52-58	5.3	131
224	Prediction of Experimental Methanol Decomposition Rates on Platinum from First Principles. *Topics in Catalysis*, **2006**, 37, 17-28	2.3	129
223	Direct time-domain observation of attosecond final-state lifetimes in photoemission from solids. *Science*, **2016**, 353, 62-7	33.3	126
222	Bismuthene for highly efficient carbon dioxide electroreduction reaction. *Nature Communications*, **2020**, 11, 1088	17.4	125
221	Facile synthesis of palladium right bipyramids and their use as seeds for overgrowth and as catalysts for formic acid oxidation. *Journal of the American Chemical Society*, **2013**, 135, 15706-9	16.4	125
220	Active sites and mechanisms for HDO decomposition over Pd catalysts. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, E1973-82	11.5	122
219	Tuning the Catalytic Activity of Core–Shell Nanoparticles for the Oxygen Reduction Reaction by Varying the Shell Thickness. *Journal of Physical Chemistry C*, **2013**, 117, 1748-1753	3.8	120
218	CO2 Hydrogenation to Formic Acid on Ni(111). *Journal of Physical Chemistry C*, **2012**, 116, 3001-3006	3.8	119
217	First Synthesis, Experimental and Theoretical Vibrational Spectra of an Oxametallacycle on a Metal Surface. *Journal of the American Chemical Society*, **1998**, 120, 3196-3204	16.4	114
216	Kinetically Relevant Steps and H2/D2 Isotope Effects in Fischer–Tropsch Synthesis on Fe and Co Catalysts. *Journal of Physical Chemistry C*, **2010**, 114, 19761-19770	3.8	97
215	A simple rule of thumb for diffusion on transition-metal surfaces. *Angewandte Chemie - International Edition*, **2006**, 45, 7046-9	16.4	96
214	A Comprehensive Study of Formic Acid Oxidation on Palladium Nanocrystals with Different Types of Facets and Twin Defects. *ChemCatChem*, **2015**, 7, 2077-2084	5.2	91
213	Surface segregation energies in low-index open surfaces of bimetallic transition metal alloys. *Surface Science*, **2009**, 603, 91-96	1.8	90
212	Microkinetic analysis and mechanism of the water gas shift reaction over copper catalysts. *Journal of Catalysis*, **2011**, 281, 1-11	7.3	89
211	Atomic and molecular adsorption on Pd(111). *Surface Science*, **2012**, 606, 1670-1679	1.8	88

210	Lattice strain effects on CO oxidation on Pt(111). *Physical Chemistry Chemical Physics*, **2006**, 8, 3369-74	3.6	85
209	Electrocatalytic Oxidation of Ammonia on Transition-Metal Surfaces: A First-Principles Study. *Journal of Physical Chemistry C*, **2015**, 119, 14692-14701	3.8	84
208	Catalytic Activity of Platinum Monolayer on Iridium and Rhenium Alloy Nanoparticles for the Oxygen Reduction Reaction. *ACS Catalysis*, **2012**, 2, 817-824	13.1	84
207	Synthesis and Characterization of Ru Cubic Nanocages with a Face-Centered Cubic Structure by Templating with Pd Nanocubes. *Nano Letters*, **2016**, 16, 5310-7	11.5	84
206	Formic acid decomposition on Au catalysts: DFT, microkinetic modeling, and reaction kinetics experiments. *AICHE Journal*, **2014**, 60, 1303-1319	3.6	78
205	Density Functional Theory Calculations for Simple Oxametallacycles:Trends across the Periodic Table. *Journal of Physical Chemistry B*, **1998**, 102, 394-399	3.4	74
204	Methane Conversion to Ethylene and Aromatics on PtSn Catalysts. *ACS Catalysis*, **2017**, 7, 2088-2100	13.1	73
203	Low-temperature CO oxidation on Ni(111) and on a Au/Ni(111) surface alloy. *ACS Nano*, **2010**, 4, 4380-7	16.7	72
202	Density functional theory studies of the adsorption of ethylene and oxygen on Pt(111) and Pt[sub 3]Sn(111). *Journal of Chemical Physics*, **2001**, 114, 4663	3.9	69
201	Mixed-metal Pt monolayer electrocatalysts with improved CO tolerance. *Journal of the American Chemical Society*, **2011**, 133, 18574-6	16.4	67
200	CO vibrational frequencies on methanol synthesis catalysts: a DFT study. *Journal of Catalysis*, **2003**, 213, 63-72	7.3	65
199	CO2 hydrogenation to formic acid on Ni(110). *Surface Science*, **2012**, 606, 1050-1055	1.8	64
198	Atomic and molecular adsorption on Ru(0001). *Surface Science*, **2013**, 614, 64-74	1.8	62
197	Reaction Kinetics of Ethylene Glycol Reforming over Platinum in the Vapor versus Aqueous Phases. *Journal of Physical Chemistry C*, **2011**, 115, 961-971	3.8	62
196	On the Mechanism of Low-Temperature CO Oxidation on Ni(111) and NiO(111) Surfaces. *Journal of Physical Chemistry C*, **2010**, 114, 21579-21584	3.8	61
195	Adsorption and dissociation of O2 on Ir(111). *Journal of Chemical Physics*, **2002**, 116, 10846-10853	3.9	61
194	Computational Methods in Heterogeneous Catalysis. *Chemical Reviews*, **2021**, 121, 1007-1048	68.1	61
193	Diffusion of N adatoms on the Fe(100) surface. *Physical Review Letters*, **2000**, 84, 4898-901	7.4	60

192	Iridium-Based Cubic Nanocages with 1.1-nm-Thick Walls: A Highly Efficient and Durable Electrocatalyst for Water Oxidation in an Acidic Medium. *Angewandte Chemie - International Edition*, **2019**, 58, 7244-7248	16.4	59
191	Density Functional Theory Calculations and Analysis of Reaction Pathways for Reduction of Nitric Oxide by Hydrogen on Pt(111). *ACS Catalysis*, **2014**, 4, 3307-3319	13.1	59
190	Atomic and molecular adsorption on Au(111). *Surface Science*, **2014**, 627, 57-69	1.8	58
189	DFT Insights into the Competitive Adsorption of Sulfur- and Nitrogen-Containing Compounds and Hydrocarbons on Co-Promoted Molybdenum Sulfide Catalysts. *ACS Catalysis*, **2016**, 6, 2904-2917	13.1	58
188	Eliminating dissolution of platinum-based electrocatalysts at the atomic scale. *Nature Materials*, **2020**, 19, 1207-1214	27	57
187	Strain-induced formation of subsurface species in transition metals. *Angewandte Chemie - International Edition*, **2004**, 43, 4296-300	16.4	56
186	Density functional theory studies of HCOOH decomposition on Pd(111). *Surface Science*, **2016**, 650, 111-120	1.8	55
185	Direct Visualization of Catalytically Active Sites at the FeO-Pt(111) Interface. *ACS Nano*, **2015**, 9, 7804-14	16.7	54
184	On the Preferred Active Sites of Promoted MoS2 for Hydrodesulfurization with Minimal Organonitrogen Inhibition. *ACS Catalysis*, **2017**, 7, 501-509	13.1	53
183	Water clustering on nanostructured iron oxide films. *Nature Communications*, **2014**, 5, 4193	17.4	53
182	Reduction of FeO/Pt(111) thin films by exposure to atomic hydrogen. *Surface Science*, **2010**, 604, 11-20	1.8	52
181	Tip-Dependent Scanning Tunneling Microscopy Imaging of Ultrathin FeO Films on Pt(111). *Journal of Physical Chemistry C*, **2011**, 115, 2089-2099	3.8	50
180	Correlating STM contrast and atomic-scale structure by chemical modification: Vacancy dislocation loops on FeO/Pt(1 1 1). *Surface Science*, **2009**, 603, L15-L18	1.8	50
179	Atomic-scale evidence for an enhanced catalytic reactivity of stretched surfaces. *Angewandte Chemie - International Edition*, **2003**, 42, 2850-3	16.4	50
178	Density-functional theory studies of acetone and propanal hydrogenation on Pt(111). *Journal of Chemical Physics*, **2002**, 116, 8973-8980	3.9	50
177	Ab initio molecular dynamics of solvation effects on reactivity at electrified interfaces. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, E4937-45	11.5	50
176	Molecular N2 chemisorption: Specific adsorption on step defect sites on Pt surfaces. *Journal of Chemical Physics*, **1999**, 111, 8651-8658	3.9	49
175	Conductance of Conjugated Molecular Wires: Length Dependence, Anchoring Groups, and Band Alignment. *Journal of Physical Chemistry C*, **2009**, 113, 20967-20973	3.8	48

174	Distinguishing attosecond electron-electron scattering and screening in transition metals. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E5300-E5307	11.5	47
173	Facile Synthesis of Ru-Based Octahedral Nanocages with Ultrathin Walls in a Face-Centered Cubic Structure. *Chemistry of Materials*, **2017**, 29, 9227-9237	9.6	45
172	Synthesis of Ru Icosahedral Nanocages with a Face-Centered-Cubic Structure and Evaluation of Their Catalytic Properties. *ACS Catalysis*, **2018**, 8, 6948-6960	13.1	45
171	HCOOH decomposition on Pt(111): A DFT study. *Surface Science*, **2016**, 648, 201-211	1.8	44
170	Transition Metal Atoms Embedded in Graphene: How Nitrogen Doping Increases CO Oxidation Activity. *ACS Catalysis*, **2019**, 9, 6864-6868	13.1	44
169	Single-atom gold oxo-clusters prepared in alkaline solutions catalyse the heterogeneous methanol self-coupling reactions. *Nature Chemistry*, **2019**, 11, 1098-1105	17.6	44
168	Structure of Stoichiometric and Oxygen-Rich Ultrathin FeO(111) Films Grown on Pd(111). *Journal of Physical Chemistry C*, **2013**, 117, 15155-15163	3.8	43
167	Understanding the Thermal Stability of Palladium-Platinum Core-Shell Nanocrystals by In Situ Transmission Electron Microscopy and Density Functional Theory. *ACS Nano*, **2017**, 11, 4571-4581	16.7	42
166	Synthesis Gas Conversion over Rh-Based Catalysts Promoted by Fe and Mn. *ACS Catalysis*, **2017**, 7, 4550-4563	13.1	42
165	The adsorption and dissociation of O 2 molecular precursors on Cu: the effect of steps. *Surface Science*, **2003**, 538, 219-232	1.8	42
164	Interaction of carbon dioxide with Cu overlayers on Pt(111). *Surface Science*, **2008**, 602, 702-711	1.8	40
163	Thermal Stability of Metal Nanocrystals: An Investigation of the Surface and Bulk Reconstructions of Pd Concave Icosahedra. *Nano Letters*, **2017**, 17, 3655-3661	11.5	39
162	Anionic Single-Atom Catalysts for CO Oxidation: Support-Independent Activity at Low Temperatures. *ACS Catalysis*, **2019**, 9, 1595-1604	13.1	39
161	Ethylene versus ethane: A DFT-based selectivity descriptor for efficient catalyst screening. *Journal of Catalysis*, **2018**, 362, 18-24	7.3	39
160	Stabilization of Copper Catalysts for Liquid-Phase Reactions by Atomic Layer Deposition. *Angewandte Chemie*, **2013**, 125, 14053-14057	3.6	39
159	Adsorbate-induced segregation in a PdAg membrane model system: Pd3Ag(1 1 1). *Catalysis Today*, **2012**, 193, 111-119	5.3	38
158	Quantum tunneling enabled self-assembly of hydrogen atoms on Cu(111). *ACS Nano*, **2012**, 6, 10115-21	16.7	37
157	Reaction Mechanism of Vapor-Phase Formic Acid Decomposition over Platinum Catalysts: DFT, Reaction Kinetics Experiments, and Microkinetic Modeling. *ACS Catalysis*, **2020**, 10, 4112-4126	13.1	36

156	Significant quantum effects in hydrogen activation. *ACS Nano*, **2014**, 8, 4827-35	16.7	35
155	Platinum Monolayer Electrocatalysts for O2 Reduction: Pt Monolayer on Carbon-Supported PdIr Nanoparticles. *Electrocatalysis*, **2010**, 1, 213-223	2.7	35
154	On the Role of Subsurface Oxygen and Ethylenedioxy in Ethylene Epoxidation on Silver. *Journal of Physical Chemistry C*, **2007**, 111, 7992-7999	3.8	35
153	Adsorption of nitrogen- and sulfur-containing compounds on NiMoS for hydrotreating reactions: A DFT and vdW-corrected study. *AICHE Journal*, **2015**, 61, 4036-4050	3.6	34
152	The addition of Sb as a surfactant to GaN growth by metal organic vapor phase epitaxy. *Journal of Applied Physics*, **2002**, 92, 2304-2309	2.5	34
151	The nature of the Fe-graphene interface at the nanometer level. *Nanoscale*, **2015**, 7, 2450-60	7.7	33
150	Step Effects on the Dissociation of NO on Close-Packed Rhodium Surfaces. *Journal of Physical Chemistry C*, **2009**, 113, 20623-20631	3.8	33
149	Nanocatalysis beyond the gold-rush era. *Angewandte Chemie - International Edition*, **2008**, 47, 7390-2	16.4	32
148	Sequential-Optimization-Based Framework for Robust Modeling and Design of Heterogeneous Catalytic Systems. *Journal of Physical Chemistry C*, **2017**, 121, 25847-25863	3.8	30
147	Facile One-Pot Synthesis of Pd@Pt1L Octahedra with Enhanced Activity and Durability toward Oxygen Reduction. *Chemistry of Materials*, **2019**, 31, 1370-1380	9.6	29
146	Correlation Between Reactivity and Oxidation State of Cobalt Oxide Catalysts for CO Preferential Oxidation. *ACS Catalysis*, **2019**, 9, 8325-8336	13.1	29
145	Stabilities of Substituted Oxametallacycle Intermediates: Implications for Regioselectivity of Epoxide Ring Opening and Olefin Epoxidation. *Journal of Physical Chemistry B*, **1999**, 103, 11169-11175	3.4	29
144	Design of Chemoresponsive Liquid Crystals through Integration of Computational Chemistry and Experimental Studies. *Chemistry of Materials*, **2017**, 29, 3563-3571	9.6	28
143	Mechanistic Studies of Oxygen Reduction by Hydrogen on PdAg(110). *ACS Catalysis*, **2013**, 3, 1622-1632	13.1	28
142	Liquid Crystals with Interfacial Ordering that Enhances Responsiveness to Chemical Targets. *Advanced Materials*, **2018**, 30, e1706707	24	28
141	Ethylene Dimerization and Oligomerization to 1-Butene and Higher Olefins with Chromium-Promoted Cobalt on Carbon Catalyst. *ACS Catalysis*, **2018**, 8, 2488-2497	13.1	27
140	Atomic and molecular adsorption on Fe(110). *Surface Science*, **2018**, 667, 54-65	1.8	27
139	Molecular and Atomic Hydrogen Interactions with Au□ Near-Surface Alloys. *Journal of Physical Chemistry C*, **2009**, 113, 1411-1417	3.8	27

138	Combining Computational Modeling with Reaction Kinetics Experiments for Elucidating the Nature of the Active Site in Catalysis. *Accounts of Chemical Research*, **2020**, 53, 1893-1904	24.3	27
137	How Noninnocent Spectator Species Improve the Oxygen Reduction Activity of Single-Atom Catalysts: Microkinetic Models from First-Principles Calculations. *ACS Catalysis*, **2020**, 10, 9129-9135	13.1	26
136	Atomic and Molecular Adsorption on Ag(111). *Journal of Physical Chemistry C*, **2019**, 123, 7551-7566	3.8	26
135	On the Structure Sensitivity of Formic Acid Decomposition on Cu Catalysts. *Topics in Catalysis*, **2016**, 59, 1580-1588	2.3	25
134	Towards first-principles molecular design of liquid crystal-based chemoresponsive systems. *Nature Communications*, **2016**, 7, 13338	17.4	25
133	Atomic and molecular adsorption on Ni(111). *Surface Science*, **2019**, 679, 240-253	1.8	25
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131	Density Functional Theory and Reaction Kinetics Studies of the Water□Gas Shift Reaction on Pt□Re Catalysts. *ChemCatChem*, **2013**, 5, 3690-3699	5.2	25
130	Effectiveness of in situ NH3 annealing treatments for the removal of oxygen from GaN surfaces. *Surface Science*, **2009**, 603, 387-399	1.8	25
129	Hydrogen on and in Selected Overlayer Near-Surface Alloys and the Effect of Subsurface Hydrogen on the Reactivity of Alloy Surfaces. *Topics in Catalysis*, **2010**, 53, 384-392	2.3	25
128	Low-Temperature Hydrogenation of Cyclohexene by Energetic Forms of Hydrogen on the Ni(100) Surface. *The Journal of Physical Chemistry*, **1995**, 99, 6270-6272		25
127	Electrocatalysis in Alkaline Media and Alkaline Membrane-Based Energy Technologies.. *Chemical Reviews*, **2022**,	68.1	25
126	Atomic and Molecular Adsorption on Cu(111). *Topics in Catalysis*, **2018**, 61, 736-750	2.3	25
125	CO-induced embedding of Pt adatoms in a partially reduced FeO(x) film on Pt(111). *Journal of the American Chemical Society*, **2011**, 133, 10692-5	16.4	24
124	Kinetically Controlled Synthesis of Pd-Cu Janus Nanocrystals with Enriched Surface Structures and Enhanced Catalytic Activities toward CO Reduction. *Journal of the American Chemical Society*, **2021**, 143, 149-162	16.4	24
123	Structure Sensitivity of Formic Acid Electrooxidation on Transition Metal Surfaces: A First-Principles Study. *Journal of the Electrochemical Society*, **2018**, 165, J3109-J3121	3.9	24
122	Computational Chemistry-Guided Design of Selective Chemoresponsive Liquid Crystals Using Pyridine and Pyrimidine Functional Groups. *Advanced Functional Materials*, **2018**, 28, 1703581	15.6	23
121	Practical Surface Treatments and Surface Chemistry of n-Type and p-Type GaN. *Journal of Electronic Materials*, **2008**, 37, 439-447	1.9	23

120	Boron Nitride-supported Sub-nanometer Pd6 Clusters for Formic Acid Decomposition: A DFT Study. *ChemCatChem*, **2017**, 9, 1610-1620	5.2	22
119	Adsorbate diffusion on transition metal nanoparticles. *Nano Letters*, **2015**, 15, 629-34	11.5	22
118	Identification of O-rich structures on platinum(111)-supported ultrathin iron oxide films. *Surface Science*, **2016**, 652, 261-268	1.8	22
117	Brønsted–Evans–Polanyi relation for CO oxidation on metal oxides following the Mars–van Krevelen mechanism. *Journal of Catalysis*, **2019**, 377, 577-581	7.3	22
116	Atomic and Molecular Adsorption on Re(0001). *Topics in Catalysis*, **2014**, 57, 54-68	2.3	22
115	Surfactant effect of Sb on GaN growth. *Journal of Crystal Growth*, **2005**, 285, 146-155	1.6	22
114	Synthesis Gas Conversion over Rh/Mo Catalysts Prepared by Atomic Layer Deposition. *ACS Catalysis* , **2019**, 9, 1810-1819	13.1	22
113	Mechanistic Study of Nitric Oxide Reduction by Hydrogen on Pt(100) (I): A DFT Analysis of the Reaction Network. *Journal of Physical Chemistry B*, **2018**, 122, 432-443	3.4	21
112	Redox-Triggered Orientational Responses of Liquid Crystals to Chlorine Gas. *Angewandte Chemie - International Edition*, **2018**, 57, 9665-9669	16.4	21
111	On the composition of bimetallic near-surface alloys in the presence of oxygen and carbon monoxide. *Catalysis Communications*, **2014**, 52, 65-71	3.2	21
110	Alignment of semiconducting graphene nanoribbons on vicinal Ge(001). *Nanoscale*, **2019**, 11, 4864-4875	7.7	20
109	Toward rational nanoparticle synthesis: predicting surface intermixing in bimetallic alloy nanocatalysts. *Nanoscale*, **2017**, 9, 15005-15017	7.7	20
108	Oxygen Reduction Reaction on Platinum-Terminated Onion-structured Alloy Catalysts. *Electrocatalysis*, **2012**, 3, 192-202	2.7	20
107	Facet-controlled Pt Ir nanocrystals with substantially enhanced activity and durability towards oxygen reduction. *Materials Today*, **2020**, 35, 69-77	21.8	20
106	The role of anions in adsorbate-induced anchoring transitions of liquid crystals on surfaces with discrete cation binding sites. *Soft Matter*, **2018**, 14, 797-805	3.6	20
105	Density functional theory study of thermodynamic and kinetic isotope effects of H2/D2 dissociative adsorption on transition metals. *Catalysis Science and Technology*, **2018**, 8, 3321-3335	5.5	19
104	Formic Acid: A Hydrogen-Bonding Cocatalyst for Formate Decomposition. *ACS Catalysis*, **2020**, 10, 10812–10825	13.1	19
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