Manos Mavrikakis

List of Publications by Year
in descending order

285	36,677	5558 82	3173 186
papers	citations	h-index	g-index

305	305	305	24182
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Highly Crystalline Multimetallic Nanoframes with Three-Dimensional Electrocatalytic Surfaces. Science, 2014, 343, 1339-1343.	6.0	2,376
2	Effect of Strain on the Reactivity of Metal Surfaces. Physical Review Letters, 1998, 81, 2819-2822.	2.9	2,001
3	Universality in Heterogeneous Catalysis. Journal of Catalysis, 2002, 209, 275-278.	3.1	1,167
4	Ruâ€“Pt coreâ€“shell nanoparticles for preferential oxidation of carbon monoxide in hydrogen. Nature Materials, 2008, 7, 333-338.	13.3	1,146
5	On the origin of the catalytic activity of gold nanoparticles for low-temperature CO oxidation. Journal of Catalysis, 2004, 223, 232-235.	3.1	1,122
6	Alloy catalysts designed from first principles. Nature Materials, 2004, 3, 810-815.	13.3	1,030
7	Controlling the Catalytic Activity of Platinum-Monolayer Electrocatalysts for Oxygen Reduction with Different Substrates. Angewandte Chemie - International Edition, 2005, 44, 2132-2135.	7.2	1,015
8	Mechanism of Methanol Synthesis on Cu through CO₂and CO Hydrogenation. ACS Catalysis, 2011, 1, 365-384.	5.5	990
9	ELECTRONICSTRUCTURE ANDCATALYSIS ONMETALSURFACES. Annual Review of Physical Chemistry, 2002, 53, 319-348.	4.8	906
10	Platinum-based nanocages with subnanometer-thick walls and well-defined, controllable facets. Science, 2015, 349, 412-416.	6.0	854
11	On the Mechanism of Low-Temperature Water Gas Shift Reaction on Copper. Journal of the American Chemical Society, 2008, 130, 1402-1414.	6.6	839
12	Platinum Monolayer Fuel Cell Electrocatalysts. Topics in Catalysis, 2007, 46, 249-262.	1.3	820
13	Making gold less noble. Catalysis Letters, 2000, 64, 101-106.	1.4	641
14	Alkali-Stabilized Pt-OH _x Species Catalyze Low-Temperature Water-Gas Shift Reactions. Science, 2010, 329, 1633-1636.	6.0	639
15	Adsorption and Dissociation of O2on Ptâ^'Co and Ptâ^'Fe Alloys. Journal of the American Chemical Society, 2004, 126, 4717-4725.	6.6	615
16	Mixed-Metal Pt Monolayer Electrocatalysts for Enhanced Oxygen Reduction Kinetics. Journal of the American Chemical Society, 2005, 127, 12480-12481.	6.6	556
17	Catalytically active Au-O(OH) _x - species stabilized by alkali ions on zeolites and mesoporous oxides. Science, 2014, 346, 1498-1501.	6.0	544
18	CO activation pathways and the mechanism of Fischerâ€“Tropsch synthesis. Journal of Catalysis, 2010, 272, 287-297.	3.1	487

#	Article	IF	Citations
19	Mechanism of the Water Gas Shift Reaction on Pt:â€‰ First Principles, Experiments, and Microkinetic Modeling. Journal of Physical Chemistry C, 2008, 112, 4608-4617.	1.5	452
20	Atomic Layer-by-Layer Deposition of Pt on Pd Nanocubes for Catalysts with Enhanced Activity and Durability toward Oxygen Reduction. Nano Letters, 2014, 14, 3570-3576.	4.5	448
21	Palladiumâ€“platinum core-shell icosahedra with substantially enhanced activity and durability towards oxygen reduction. Nature Communications, 2015, 6, 7594.	5.8	440
22	Competitive Paths for Methanol Decomposition on Pt(111). Journal of the American Chemical Society, 2004, 126, 3910-3919.	6.6	389
23	Hydrogen adsorption, absorption and diffusion on and in transition metal surfaces: A DFT study. Surface Science, 2012, 606, 679-689.	0.8	380
24	Oxygenate reaction pathways on transition metal surfaces. Journal of Molecular Catalysis A, 1998, 131, 135-147.	4.8	350
25	Surface and Subsurface Hydrogen:Â Adsorption Properties on Transition Metals and Near-Surface Alloys. Journal of Physical Chemistry B, 2005, 109, 3460-3471.	1.2	343
26	Adsorption and Dissociation of O2on Gold Surfaces:Â Effect of Steps and Strain. Journal of Physical Chemistry B, 2003, 107, 9298-9307.	1.2	322
27	A First-Principles Study of Methanol Decomposition on Pt(111). Journal of the American Chemical Society, 2002, 124, 7193-7201.	6.6	316
28	DFT studies for cleavage of C$z.sbnd;C and C$z.sbnd;O bonds in surface species derived from ethanol on Pt(111). Journal of Catalysis, 2003, 218, 178-190.	3.1	289
29	Bismuthene for highly efficient carbon dioxide electroreduction reaction. Nature Communications, 2020, 11, 1088.	5.8	278
30	Modeling Ethanol Decomposition on Transition Metals: A Combined Application of Scaling and BrÃ¸nstedâ€“Evansâ€“Polanyi Relations. Journal of the American Chemical Society, 2009, 131, 5809-5815.	6.6	275
31	Preferential CO Oxidation in Hydrogen: Reactivity of Coreâ€“Shell Nanoparticles. Journal of the American Chemical Society, 2010, 132, 7418-7428.	6.6	258
32	Atomic and molecular adsorption on Pt(111). Surface Science, 2005, 587, 159-174.	0.8	247
33	Water-Mediated Proton Hopping on an Iron Oxide Surface. Science, 2012, 336, 889-893.	6.0	242
34	Why Au and Cu Are More Selective Than Pt for Preferential Oxidation of CO at Low Temperature. Catalysis Letters, 2004, 93, 93-100.	1.4	238
35	A Cu/Pt Near-Surface Alloy for Waterâ€“Gas Shift Catalysis. Journal of the American Chemical Society, 2007, 129, 6485-6490.	6.6	233
36	Platinum monolayer electrocatalysts for oxygen reduction. Electrochimica Acta, 2007, 52, 2257-2263.	2.6	230

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37	Molecular-level descriptions of surface chemistry in kinetic models using density functional theory. Chemical Engineering Science, 2004, 59, 4679-4691.	1.9	227
38	Improving Electrocatalysts for O₂Reduction by Fine-Tuning the Ptâ^'Support Interaction: Pt Monolayer on the Surfaces of a Pd₃Fe(111) Single-Crystal Alloy. Journal of the American Chemical Society, 2009, 131, 12755-12762.	6.6	224
39	Trends in low-temperature water?gas shift reactivity on transition metals. Journal of Catalysis, 2005, 229, 265-275.	3.1	213
40	Atomic Layer-by-Layer Deposition of Platinum on Palladium Octahedra for Enhanced Catalysts toward the Oxygen Reduction Reaction. ACS Nano, 2015, 9, 2635-2647.	7.3	209
41	Atomic and molecular adsorption on Rh(111). Journal of Chemical Physics, 2002, 117, 6737-6744.	1.2	204
42	Improved oxygen reduction reactivity of platinum monolayers on transition metal surfaces. Surface Science, 2008, 602, L89-L94.	0.8	204
43	Structure Sensitivity of Methanol Electrooxidation on Transition Metals. Journal of the American Chemical Society, 2009, 131, 14381-14389.	6.6	203
44	Bimetallic and Ternary Alloys for Improved Oxygen Reduction Catalysis. Topics in Catalysis, 2007, 46, 276-284.	1.3	202
45	Computational Methods in Heterogeneous Catalysis. Chemical Reviews, 2021, 121, 1007-1048.	23.0	198
46	Electrocatalysis in Alkaline Media and Alkaline Membrane-Based Energy Technologies. Chemical Reviews, 2022, 122, 6117-6321.	23.0	195
47	Methanol Decomposition on Cu(111): A DFT Study. Journal of Catalysis, 2002, 208, 291-300.	3.1	190
48	Trends in Formic Acid Decomposition on Model Transition Metal Surfaces: A Density Functional Theory study. ACS Catalysis, 2014, 4, 4434-4445.	5.5	190
49	Partial and complete reduction of O2 by hydrogen on transition metal surfaces. Surface Science, 2010, 604, 1565-1575.	0.8	189
50	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.	0.8	183
51	Direct time-domain observation of attosecond final-state lifetimes in photoemission from solids. Science, 2016, 353, 62-67.	6.0	181
52	Adsorption and dissociation of O2 on Cu(): thermochemistry, reaction barrier and the effect of strain. Surface Science, 2001, 494, 131-144.	0.8	175
53	Active sites and mechanisms for H ₂ O ₂ decomposition over Pd catalysts. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E1973-82.	3.3	171
54	Reactivity descriptors for direct methanol fuel cell anode catalysts. Surface Science, 2008, 602, 3424-3431.	0.8	168

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55	Stabilization of Copper Catalysts for Liquidâ€Phase Reactions by Atomic Layer Deposition. Angewandte Chemie - International Edition, 2013, 52, 13808-13812.	7.2	162
56	Bifunctional anode catalysts for direct methanol fuel cells. Energy and Environmental Science, 2012, 5, 8335.	15.6	157
57	Structure Sensitivity of CO Dissociation on Rh Surfaces. Catalysis Letters, 2002, 81, 153-156.	1.4	153
58	Effect of Subsurface Oxygen on the Reactivity of the Ag(111) Surface. Journal of the American Chemical Society, 2005, 127, 12823-12827.	6.6	151
59	Synthesis and Characterization of Ptâ€“Ag Alloy Nanocages with Enhanced Activity and Durability toward Oxygen Reduction. Nano Letters, 2016, 16, 6644-6649.	4.5	150
60	Near-surface alloys for hydrogen fuel cell applications. Catalysis Today, 2006, 111, 52-58.	2.2	148
61	Atomic and Molecular Adsorption on Ir(111). Journal of Physical Chemistry B, 2004, 108, 987-994.	1.2	145
62	CO₂ Hydrogenation to Formic Acid on Ni(111). Journal of Physical Chemistry C, 2012, 116, 3001-3006.	1.5	141
63	Prediction of Experimental Methanol Decomposition Rates on Platinum from First Principles. Topics in Catalysis, 2006, 37, 17-28.	1.3	140
64	Tuning the Catalytic Activity of Ru@Pt Coreâ€“Shell Nanoparticles for the Oxygen Reduction Reaction by Varying the Shell Thickness. Journal of Physical Chemistry C, 2013, 117, 1748-1753.	1.5	140
65	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, 15706-15709.	6.6	139
66	Electrocatalytic Oxidation of Ammonia on Transition-Metal Surfaces: A First-Principles Study. Journal of Physical Chemistry C, 2015, 119, 14692-14701.	1.5	137
67	First Synthesis, Experimental and Theoretical Vibrational Spectra of an Oxametallacycle on a Metal Surface. Journal of the American Chemical Society, 1998, 120, 3196-3204.	6.6	129
68	Eliminating dissolution of platinum-based electrocatalysts at the atomic scale. Nature Materials, 2020, 19, 1207-1214.	13.3	127
69	Atomic and molecular adsorption on Pd(111). Surface Science, 2012, 606, 1670-1679.	0.8	119
70	A Comprehensive Study of Formic Acid Oxidation on Palladium Nanocrystals with Different Types of Facets and Twin Defects. ChemCatChem, 2015, 7, 2077-2084.	1.8	111
71	Kinetically Relevant Steps and H₂/D₂Isotope Effects in Fischerâ€“Tropsch Synthesis on Fe and Co Catalysts. Journal of Physical Chemistry C, 2010, 114, 19761-19770.	1.5	110
72	Synthesis and Characterization of Ru Cubic Nanocages with a Face-Centered Cubic Structure by Templating with Pd Nanocubes. Nano Letters, 2016, 16, 5310-5317.	4.5	110

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73	A Simple Rule of Thumb for Diffusion on Transition-Metal Surfaces. Angewandte Chemie - International Edition, 2006, 45, 7046-7049.	7.2	109
74	Steam-created grain boundaries for methane Câ€“H activation in palladium catalysts. Science, 2021, 373, 1518-1523.	6.0	105
75	Microkinetic analysis and mechanism of the water gas shift reaction over copper catalysts. Journal of Catalysis, 2011, 281, 1-11.	3.1	100
76	Surface segregation energies in low-index open surfaces of bimetallic transition metal alloys. Surface Science, 2009, 603, 91-96.	0.8	98
77	Lattice strain effects on CO oxidation on Pt(111). Physical Chemistry Chemical Physics, 2006, 8, 3369.	1.3	96
78	Catalytic Activity of Platinum Monolayer on Iridium and Rhenium Alloy Nanoparticles for the Oxygen Reduction Reaction. ACS Catalysis, 2012, 2, 817-824.	5.5	94
79	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.	5.5	93
80	Methane Conversion to Ethylene and Aromatics on PtSn Catalysts. ACS Catalysis, 2017, 7, 2088-2100.	5.5	93
81	Iridiumâ€Based Cubic Nanocages with 1.1â€nmâ€Thick Walls: A Highly Efficient and Durable Electrocatalyst for Water Oxidation in an Acidic Medium. Angewandte Chemie - International Edition, 2019, 58, 7244-7248.	7.2	89
82	Formic acid decomposition on Au catalysts: DFT, microkinetic modeling, and reaction kinetics experiments. AIChE Journal, 2014, 60, 1303-1319.	1.8	87
83	Density Functional Theory Calculations for Simple Oxametallacycles:Â Trends across the Periodic Table. Journal of Physical Chemistry B, 1998, 102, 394-399.	1.2	84
84	Single-atom gold oxo-clusters prepared in alkaline solutions catalyse the heterogeneous methanol self-coupling reactions. Nature Chemistry, 2019, 11, 1098-1105.	6.6	82
85	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.	1.2	80
86	Low-Temperature CO Oxidation on Ni(111) and on a Au/Ni(111) Surface Alloy. ACS Nano, 2010, 4, 4380-4387.	7.3	80
87	Atomic and molecular adsorption on Au(111). Surface Science, 2014, 627, 57-69.	0.8	78
88	On the Preferred Active Sites of Promoted MoS₂ for Hydrodesulfurization with Minimal Organonitrogen Inhibition. ACS Catalysis, 2017, 7, 501-509.	5.5	78
89	CO vibrational frequencies on methanol synthesis catalysts: a DFT study. Journal of Catalysis, 2003, 213, 63-72.	3.1	77
90	Mixed-Metal Pt Monolayer Electrocatalysts with Improved CO Tolerance. Journal of the American Chemical Society, 2011, 133, 18574-18576.	6.6	77

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91	Kinetically Controlled Synthesis of Pdâ€“Cu Janus Nanocrystals with Enriched Surface Structures and Enhanced Catalytic Activities toward CO₂ Reduction. Journal of the American Chemical Society, 2021, 143, 149-162.	6.6	77
92	CO2 hydrogenation to formic acid on Ni(110). Surface Science, 2012, 606, 1050-1055.	0.8	76
93	Transition Metal Atoms Embedded in Graphene: How Nitrogen Doping Increases CO Oxidation Activity. ACS Catalysis, 2019, 9, 6864-6868.	5.5	72
94	On the Mechanism of Low-Temperature CO Oxidation on Ni(111) and NiO(111) Surfaces. Journal of Physical Chemistry C, 2010, 114, 21579-21584.	1.5	71
95	Atomic and molecular adsorption on Ru(0001). Surface Science, 2013, 614, 64-74.	0.8	71
96	Density functional theory studies of HCOOH decomposition on Pd(111). Surface Science, 2016, 650, 111-120.	0.8	70
97	Reaction Kinetics of Ethylene Glycol Reforming over Platinum in the Vapor versus Aqueous Phases. Journal of Physical Chemistry C, 2011, 115, 961-971.	1.5	68
98	Adsorption and dissociation of O2 on Ir(111). Journal of Chemical Physics, 2002, 116, 10846-10853.	1.2	67
99	Direct Visualization of Catalytically Active Sites at the FeOâ€“Pt(111) Interface. ACS Nano, 2015, 9, 7804-7814.	7.3	67
100	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.	5.5	66
101	Synthesis of Ru Icosahedral Nanocages with a Face-Centered-Cubic Structure and Evaluation of Their Catalytic Properties. ACS Catalysis, 2018, 8, 6948-6960.	5.5	66
102	Diffusion of N Adatoms on the Fe(100) Surface. Physical Review Letters, 2000, 84, 4898-4901.	2.9	65
103	Water clustering on nanostructured iron oxide films. Nature Communications, 2014, 5, 4193.	5.8	65
104	Strain-Induced Formation of Subsurface Species in Transition Metals. Angewandte Chemie - International Edition, 2004, 43, 4296-4300.	7.2	64
105	Atomic-Scale Evidence for an Enhanced Catalytic Reactivity of Stretched Surfaces. Angewandte Chemie - International Edition, 2003, 42, 2850-2853.	7.2	60
106	Reduction of FeO/Pt(111) thin films by exposure to atomic hydrogen. Surface Science, 2010, 604, 11-20.	0.8	58
107	Correlation Between Reactivity and Oxidation State of Cobalt Oxide Catalysts for CO Preferential Oxidation. ACS Catalysis, 2019, 9, 8325-8336.	5.5	58
108	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.	3.3	57

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109	Molecular N2 chemisorptionâ€"specific adsorption on step defect sites on Pt surfaces. Journal of Chemical Physics, 1999, 111, 8651-8658.	1.2	56
110	Tip-Dependent Scanning Tunneling Microscopy Imaging of Ultrathin FeO Films on Pt(111). Journal of Physical Chemistry C, 2011, 115, 2089-2099.	1.5	55
111	Facile Synthesis of Ru-Based Octahedral Nanocages with Ultrathin Walls in a Face-Centered Cubic Structure. Chemistry of Materials, 2017, 29, 9227-9237.	3.2	55
112	Distinguishing attosecond electronâ€"electron scattering and screening in transition metals. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E5300-E5307.	3.3	55
113	Density-functional theory studies of acetone and propanal hydrogenation on Pt(111). Journal of Chemical Physics, 2002, 116, 8973-8980.	1.2	54
114	HCOOH decomposition on Pt(111): A DFT study. Surface Science, 2016, 648, 201-211.	0.8	54
115	Anionic Single-Atom Catalysts for CO Oxidation: Support-Independent Activity at Low Temperatures. ACS Catalysis, 2019, 9, 1595-1604.	5.5	54
116	A completely precious metalâ€"free alkaline fuel cell with enhanced performance using a carbon-coated nickel anode. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2119883119.	3.3	54
117	Correlating STM contrast and atomic-scale structure by chemical modification: Vacancy dislocation loops on FeO/Pt(111). Surface Science, 2009, 603, L15-L18.	0.8	53
118	Understanding the Thermal Stability of Palladiumâ€"Platinum Coreâ€"Shell Nanocrystals by In Situ Transmission Electron Microscopy and Density Functional Theory. ACS Nano, 2017, 11, 4571-4581.	7.3	53
119	Combining Computational Modeling with Reaction Kinetics Experiments for Elucidating the In Situ Nature of the Active Site in Catalysis. Accounts of Chemical Research, 2020, 53, 1893-1904.	7.6	53
120	Conductance of Conjugated Molecular Wires: Length Dependence, Anchoring Groups, and Band Alignment. Journal of Physical Chemistry C, 2009, 113, 20967-20973.	1.5	52
121	Structure of Stoichiometric and Oxygen-Rich Ultrathin FeO(111) Films Grown on Pd(111). Journal of Physical Chemistry C, 2013, 117, 15155-15163.	1.5	52
122	Ethylene versus ethane: A DFT-based selectivity descriptor for efficient catalyst screening. Journal of Catalysis, 2018, 362, 18-24.	3.1	52
123	A search engine for catalysts. Nature Materials, 2006, 5, 847-848.	13.3	51
124	Synthesis Gas Conversion over Rh-Based Catalysts Promoted by Fe and Mn. ACS Catalysis, 2017, 7, 4550-4563.	5.5	51
125	Reaction Mechanism of Vapor-Phase Formic Acid Decomposition over Platinum Catalysts: DFT, Reaction Kinetics Experiments, and Microkinetic Modeling. ACS Catalysis, 2020, 10, 4112-4126.	5.5	51
126	Atomic and molecular adsorption on Fe(110). Surface Science, 2018, 667, 54-65.	0.8	49

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127	The adsorption and dissociation of O 2 molecular precursors on Cu: the effect of steps. Surface Science, 2003, 538, 219-232.	0.8	47
128	Quantum Tunneling Enabled Self-Assembly of Hydrogen Atoms on Cu(111). ACS Nano, 2012, 6, 10115-10121.	7.3	45
129	Atomic and Molecular Adsorption on Cu(111). Topics in Catalysis, 2018, 61, 736-750.	1.3	45
130	Facet-controlled Ptâ€“Ir nanocrystals with substantially enhanced activity and durability towards oxygen reduction. Materials Today, 2020, 35, 69-77.	8.3	45
131	Interaction of carbon dioxide with Cu overlayers on Pt(111). Surface Science, 2008, 602, 702-711.	0.8	44
132	Significant Quantum Effects in Hydrogen Activation. ACS Nano, 2014, 8, 4827-4835.	7.3	44
133	The nature of the Feâ€“graphene interface at the nanometer level. Nanoscale, 2015, 7, 2450-2460.	2.8	44
134	Site-dependent reactivity of MoS2 nanoparticles in hydrodesulfurization of thiophene. Nature Communications, 2020, 11, 4369.	5.8	44
135	Thermal Stability of Metal Nanocrystals: An Investigation of the Surface and Bulk Reconstructions of Pd Concave Icosahedra. Nano Letters, 2017, 17, 3655-3661.	4.5	43
136	Liquid Crystals with Interfacial Ordering that Enhances Responsiveness to Chemical Targets. Advanced Materials, 2018, 30, e1706707.	11.1	43
137	Adsorbate-induced segregation in a PdAg membrane model system: Pd3Ag(111). Catalysis Today, 2012, 193, 111-119.	2.2	42
138	Sequential-Optimization-Based Framework for Robust Modeling and Design of Heterogeneous Catalytic Systems. Journal of Physical Chemistry C, 2017, 121, 25847-25863.	1.5	42
139	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.	5.5	42
140	Solution-Phase Synthesis of PdH_{0.706} Nanocubes with Enhanced Stability and Activity toward Formic Acid Oxidation. Journal of the American Chemical Society, 2022, 144, 2556-2568.	6.6	42
141	Atomic and molecular adsorption on Ni(111). Surface Science, 2019, 679, 240-253.	0.8	41
142	Facile One-Pot Synthesis of Pd@Pt_{1L} Octahedra with Enhanced Activity and Durability toward Oxygen Reduction. Chemistry of Materials, 2019, 31, 1370-1380.	3.2	41
143	On the Role of Subsurface Oxygen and Ethylenedioxy in Ethylene Epoxidation on Silver. Journal of Physical Chemistry C, 2007, 111, 7992-7999.	1.5	40
144	Platinum Monolayer Electrocatalysts for O2 Reduction: Pt Monolayer on Carbon-Supported PdIr Nanoparticles. Electrocatalysis, 2010, 1, 213-223.	1.5	40

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145	Adsorption of nitrogenâ€•and sulfurâ€•containing compounds on NiMoS for hydrotreating reactions: A DFT and vdWâ€•corrected study. AIChE Journal, 2015, 61, 4036-4050.	1.8	39
146	Structure Sensitivity of Formic Acid Electrooxidation on Transition Metal Surfaces: A First-Principles Study. Journal of the Electrochemical Society, 2018, 165, J3109-J3121.	1.3	39
147	Redoxâ€Triggered Orientational Responses of Liquid Crystals to Chlorine Gas. Angewandte Chemie - International Edition, 2018, 57, 9665-9669.	7.2	39
148	Atomic and Molecular Adsorption on Ag(111). Journal of Physical Chemistry C, 2019, 123, 7551-7566.	1.5	39
149	On the Structure Sensitivity of Formic Acid Decomposition on Cu Catalysts. Topics in Catalysis, 2016, 59, 1580-1588.	1.3	37
150	Ethylene Dimerization and Oligomerization to 1-Butene and Higher Olefins with Chromium-Promoted Cobalt on Carbon Catalyst. ACS Catalysis, 2018, 8, 2488-2497.	5.5	37
151	Step Effects on the Dissociation of NO on Close-Packed Rhodium Surfaces. Journal of Physical Chemistry C, 2009, 113, 20623-20631.	1.5	36
152	Formic Acid: A Hydrogen-Bonding Cocatalyst for Formate Decomposition. ACS Catalysis, 2020, 10, 10812-10825.	5.5	36
153	The addition of Sb as a surfactant to GaN growth by metal organic vapor phase epitaxy. Journal of Applied Physics, 2002, 92, 2304-2309.	1.1	35
154	Nanocatalysis Beyond the Goldâ€Rush Era. Angewandte Chemie - International Edition, 2008, 47, 7390-7392.	7.2	34
155	Towards first-principles molecular design of liquid crystal-based chemoresponsive systems. Nature Communications, 2016, 7, 13338.	5.8	34
156	Design of Chemoresponsive Liquid Crystals through Integration of Computational Chemistry and Experimental Studies. Chemistry of Materials, 2017, 29, 3563-3571.	3.2	33
157	BrÃ¸nstedâ€“Evansâ€“Polanyi relation for CO oxidation on metal oxides following the Marsâ€“van Krevelen mechanism. Journal of Catalysis, 2019, 377, 577-581.	3.1	33
158	Synthesis Gas Conversion over Rh/Mo Catalysts Prepared by Atomic Layer Deposition. ACS Catalysis, 2019, 9, 1810-1819.	5.5	33
159	Janus Nanocages of Platinumâ€Group Metals and Their Use as Effective Dualâ€Electrocatalysts. Angewandte Chemie - International Edition, 2021, 60, 10384-10392.	7.2	33
160	Introduction: Advanced Materials and Methods for Catalysis and Electrocatalysis by Transition Metals. Chemical Reviews, 2021, 121, 563-566.	23.0	33
161	Mechanistic Studies of Oxygen Reduction by Hydrogen on PdAg(110). ACS Catalysis, 2013, 3, 1622-1632.	5.5	32
162	An Adsorption Study of CH₄ on ZSM-5, MOR, and ZSM-12 Zeolites. Journal of Physical Chemistry C, 2015, 119, 28970-28978.	1.5	32

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163	Structure sensitivity of ammonia electro-oxidation on transition metal surfaces: A first-principles study. Journal of Catalysis, 2021, 397, 137-147.	3.1	31
164	Thermodynamics Perspective on the Stepwise Conversion of Methane to Methanol over Cu-Exchanged SSZ-13. ACS Catalysis, 2021, 11, 7719-7734.	5.5	31
165	Stabilities of Substituted Oxametallacycle Intermediates:Â Implications for Regioselectivity of Epoxide Ring Opening and Olefin Epoxidation. Journal of Physical Chemistry B, 1999, 103, 11169-11175.	1.2	30
166	Areas of opportunity related to design of chemical and biological sensors based on liquid crystals. Liquid Crystals Today, 2020, 29, 24-35.	2.3	30
167	Effectiveness of in situ NH3 annealing treatments for the removal of oxygen from GaN surfaces. Surface Science, 2009, 603, 387-399.	0.8	29
168	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.	1.2	29
169	Density Functional Theory and Reaction Kinetics Studies of the Waterâ€“Gas Shift Reaction on Ptâ€“Re Catalysts. ChemCatChem, 2013, 5, 3690-3699.	1.8	28
170	Atomic and Molecular Adsorption on Re(0001). Topics in Catalysis, 2014, 57, 54-68.	1.3	28
171	Molecular and Atomic Hydrogen Interactions with Auâ^'Ir Near-Surface Alloys. Journal of Physical Chemistry C, 2009, 113, 1411-1417.	1.5	27
172	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.	1.3	27
173	CO-Induced Embedding of Pt Adatoms in a Partially Reduced FeOxFilm on Pt(111). Journal of the American Chemical Society, 2011, 133, 10692-10695.	6.6	27
174	Identification of O-rich structures on platinum(111)-supported ultrathin iron oxide films. Surface Science, 2016, 652, 261-268.	0.8	27
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