Jens Norskov

List of Publications by Year
in descending order

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677 papers	198,573 citations	16 205 h-index	31 428 g-index
736 all docs	736 docs citations	736 times ranked	65887 citing authors

#	Article	IF	Citations
1	Origin of the Overpotential for Oxygen Reduction at a Fuel-Cell Cathode. Journal of Physical Chemistry B, 2004, 108, 17886-17892.	1.2	8,672
2	Combining theory and experiment in electrocatalysis: Insights into materials design. Science, 2017, 355, .	6.0	7,837
3	Improved adsorption energetics within density-functional theory using revised Perdew-Burke-Ernzerhof functionals. Physical Review B, 1999, 59, 7413-7421.	1.1	6,206
4	Trends in the Exchange Current for Hydrogen Evolution. Journal of the Electrochemical Society, 2005, 152, J23.	1.3	4,054
5	Biomimetic Hydrogen Evolution:Â MoS2Nanoparticles as Catalyst for Hydrogen Evolution. Journal of the American Chemical Society, 2005, 127, 5308-5309.	6.6	3,497
6	Computational high-throughput screening of electrocatalytic materials for hydrogen evolution. Nature Materials, 2006, 5, 909-913.	13.3	3,305
7	Universality in Oxygen Evolution Electrocatalysis on Oxide Surfaces. ChemCatChem, 2011, 3, 1159-1165.	1.8	3,208
8	Towards the computational design of solid catalysts. Nature Chemistry, 2009, 1, 37-46.	6.6	3,184
9	Why gold is the noblest of all the metals. Nature, 1995, 376, 238-240.	13.7	2,902
10	Alloys of platinum and early transition metals as oxygen reduction electrocatalysts. Nature Chemistry, 2009, 1, 552-556.	6.6	2,716
11	Progress and Perspectives of Electrochemical CO₂ Reduction on Copper in Aqueous Electrolyte. Chemical Reviews, 2019, 119, 7610-7672.	23.0	2,708
12	How copper catalyzes the electroreduction of carbon dioxide into hydrocarbon fuels. Energy and Environmental Science, 2010, 3, 1311.	15.6	2,682
13	Electrolysis of water on oxide surfaces. Journal of Electroanalytical Chemistry, 2007, 607, 83-89.	1.9	2,277
14	Electronic factors determining the reactivity of metal surfaces. Surface Science, 1995, 343, 211-220.	0.8	2,087
15	Activating and optimizing MoS2 basal planes for hydrogen evolution through the formation of strained sulphur vacancies. Nature Materials, 2016, 15, 48-53.	13.3	2,021
16	The Active Site of Methanol Synthesis over Cu/ZnO/Al ₂ O ₃ Industrial Catalysts. Science, 2012, 336, 893-897.	6.0	2,018
17	Identification of Highly Active Fe Sites in (Ni,Fe)OOH for Electrocatalytic Water Splitting. Journal of the American Chemical Society, 2015, 137, 1305-1313.	6.6	2,018
18	Effect of Strain on the Reactivity of Metal Surfaces. Physical Review Letters, 1998, 81, 2819-2822.	2.9	2,001

#	Article	IF	Citations
19	Changing the Activity of Electrocatalysts for Oxygen Reduction by Tuning the Surface Electronic Structure. Angewandte Chemie - International Edition, 2006, 45, 2897-2901.	7.2	1,685
20	Understanding Catalytic Activity Trends in the Oxygen Reduction Reaction. Chemical Reviews, 2018, 118, 2302-2312.	23.0	1,666
21	Density functional theory in surface chemistry and catalysis. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 937-943.	3.3	1,644
22	A highly active and stable IrO _x /SrIrO ₃ catalyst for the oxygen evolution reaction. Science, 2016, 353, 1011-1014.	6.0	1,606
23	Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method. Journal of Physics Condensed Matter, 2010, 22, 253202.	0.7	1,451
24	Electrolysis of water on (oxidized) metal surfaces. Chemical Physics, 2005, 319, 178-184.	0.9	1,383
25	The BrÃ¸nstedâ€“Evansâ€“Polanyi relation and the volcano curve in heterogeneous catalysis. Journal of Catalysis, 2004, 224, 206-217.	3.1	1,348
26	Atomic-scale imaging of carbon nanofibre growth. Nature, 2004, 427, 426-429.	13.7	1,318
27	CO Chemisorption at Metal Surfaces and Overlayers. Physical Review Letters, 1996, 76, 2141-2144.	2.9	1,293
28	From the Sabatier principle to a predictive theory of transition-metal heterogeneous catalysis. Journal of Catalysis, 2015, 328, 36-42.	3.1	1,271
29	Scaling Properties of Adsorption Energies for Hydrogen-Containing Molecules on Transition-Metal Surfaces. Physical Review Letters, 2007, 99, 016105.	2.9	1,270
30	Activity Descriptors for CO₂ Electroreduction to Methane on Transition-Metal Catalysts. Journal of Physical Chemistry Letters, 2012, 3, 251-258.	2.1	1,250
31	Role of Strain and Ligand Effects in the Modification of the Electronic and Chemical Properties of Bimetallic Surfaces. Physical Review Letters, 2004, 93, 156801.	2.9	1,224
32	A theoretical evaluation of possible transition metal electro-catalysts for N₂reduction. Physical Chemistry Chemical Physics, 2012, 14, 1235-1245.	1.3	1,184
33	Modification of the surface electronic and chemical properties of Pt(111) by subsurface 3d transition metals. Journal of Chemical Physics, 2004, 120, 10240-10246.	1.2	1,181
34	Universality in Heterogeneous Catalysis. Journal of Catalysis, 2002, 209, 275-278.	3.1	1,167
35	Surface electronic structure and reactivity of transition and noble metals1Communication presented at the First Francqui Colloquium, Brussels, 19â€“20 February 1996.1. Journal of Molecular Catalysis A, 1997, 115, 421-429.	4.8	1,166
36	Materials for solar fuels and chemicals. Nature Materials, 2017, 16, 70-81.	13.3	1,163

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37	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
38	High-efficiency oxygen reduction to hydrogen peroxide catalysed by oxidized carbon materials. Nature Catalysis, 2018, 1, 156-162.	16.1	1,120
39	Ammonia Synthesis from First-Principles Calculations. Science, 2005, 307, 555-558.	6.0	1,109
40	Theoretical Investigation of the Activity of Cobalt Oxides for the Electrochemical Oxidation of Water. Journal of the American Chemical Society, 2013, 135, 13521-13530.	6.6	1,093
41	Density functionals for surface science: Exchange-correlation model development with Bayesian error estimation. Physical Review B, 2012, 85, .	1.1	1,087
42	Catalytic activity of Au nanoparticles. Nano Today, 2007, 2, 14-18.	6.2	1,025
43	The Challenge of Electrochemical Ammonia Synthesis: A New Perspective on the Role of Nitrogen Scaling Relations. ChemSusChem, 2015, 8, 2180-2186.	3.6	1,018
44	A rigorous electrochemical ammonia synthesis protocol with quantitative isotope measurements. Nature, 2019, 570, 504-508.	13.7	1,006
45	Twin Problems of Interfacial Carbonate Formation in Nonaqueous Liâ€“O₂ Batteries. Journal of Physical Chemistry Letters, 2012, 3, 997-1001.	2.1	992
46	Modeling the Electrochemical Hydrogen Oxidation and Evolution Reactions on the Basis of Density Functional Theory Calculations. Journal of Physical Chemistry C, 2010, 114, 18182-18197.	1.5	990
47	Identification of Non-Precious Metal Alloy Catalysts for Selective Hydrogenation of Acetylene. Science, 2008, 320, 1320-1322.	6.0	984
48	Steam Reforming and Graphite Formation on Ni Catalysts. Journal of Catalysis, 2002, 209, 365-384.	3.1	980
49	Ammonia for hydrogen storage: challenges and opportunities. Journal of Materials Chemistry, 2008, 18, 2304.	6.7	966
50	Design of a Surface Alloy Catalyst for Steam Reforming. Science, 1998, 279, 1913-1915.	6.0	951
51	ELECTRONICSTRUCTURE ANDCATALYSIS ONMETALSURFACES. Annual Review of Physical Chemistry, 2002, 53, 319-348.	4.8	906
52	Surface segregation energies in transition-metal alloys. Physical Review B, 1999, 59, 15990-16000.	1.1	902
53	Oxygen Vacancies as Active Sites for Water Dissociation on RutileTiO2(110). Physical Review Letters, 2001, 87, 266104.	2.9	884
54	Interatomic interactions in the effective-medium theory. Physical Review B, 1987, 35, 7423-7442.	1.1	868

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55	Discovery of a Ni-Ga catalyst for carbon dioxide reduction to methanol. Nature Chemistry, 2014, 6, 320-324.	6.6	865
56	Designing an improved transition metal phosphide catalyst for hydrogen evolution using experimental and theoretical trends. Energy and Environmental Science, 2015, 8, 3022-3029.	15.6	851
57	Atomic-Scale Structure of Single-LayerMoS2Nanoclusters. Physical Review Letters, 2000, 84, 951-954.	2.9	801
58	Hydrogen evolution on nano-particulate transition metal sulfides. Faraday Discussions, 2008, 140, 219-231.	1.6	732
59	Catalytic CO Oxidation by a Gold Nanoparticle:â€‰ A Density Functional Study. Journal of the American Chemical Society, 2002, 124, 11262-11263.	6.6	718
60	Role of Steps inN2Activation on Ru(0001). Physical Review Letters, 1999, 83, 1814-1817.	2.9	706
61	The nature of the active site in heterogeneous metal catalysis. Chemical Society Reviews, 2008, 37, 2163.	18.7	703
62	Electrochemical Ammonia Synthesisâ€”The Selectivity Challenge. ACS Catalysis, 2017, 7, 706-709.	5.5	689
63	Density functional theory calculations for the hydrogen evolution reaction in an electrochemical double layer on the Pt(111) electrode. Physical Chemistry Chemical Physics, 2007, 9, 3241-3250.	1.3	678
64	Tuning the MoS₂ Edge-Site Activity for Hydrogen Evolution via Support Interactions. Nano Letters, 2014, 14, 1381-1387.	4.5	660
65	The CO/Pt(111) Puzzle. Journal of Physical Chemistry B, 2001, 105, 4018-4025.	1.2	642
66	Making gold less noble. Catalysis Letters, 2000, 64, 101-106.	1.4	641
67	Understanding Selectivity for the Electrochemical Reduction of Carbon Dioxide to Formic Acid and Carbon Monoxide on Metal Electrodes. ACS Catalysis, 2017, 7, 4822-4827.	5.5	637
68	Catalyst Design by Interpolation in the Periodic Table:Â Bimetallic Ammonia Synthesis Catalysts. Journal of the American Chemical Society, 2001, 123, 8404-8405.	6.6	631
69	Theoretical Insights into a CO Dimerization Mechanism in CO₂ Electroreduction. Journal of Physical Chemistry Letters, 2015, 6, 2032-2037.	2.1	606
70	Understanding Trends in the Electrocatalytic Activity of Metals and Enzymes for CO₂ Reduction to CO. Journal of Physical Chemistry Letters, 2013, 4, 388-392.	2.1	604
71	Bioinspired molecular co-catalysts bonded to a silicon photocathode for solar hydrogen evolution. Nature Materials, 2011, 10, 434-438.	13.3	600
72	Metal ion cycling of Cu foil for selective Câ€“C coupling in electrochemical CO2 reduction. Nature Catalysis, 2018, 1, 111-119.	16.1	600

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73	Transition-metal doped edge sites in vertically aligned MoS2 catalysts for enhanced hydrogen evolution. Nano Research, 2015, 8, 566-575.	5.8	594
74	Hydrogen and synthesis gas by steam- and C02 reforming. Advances in Catalysis, 2002, 47, 65-139.	0.1	593
75	Oxidation and Photo-Oxidation of Water on TiO₂Surface. Journal of Physical Chemistry C, 2008, 112, 9872-9879.	1.5	587
76	The BrÃ¸nstedâ€“Evansâ€“Polanyi Relation and the Volcano Plot for Ammonia Synthesis over Transition Metal Catalysts. Journal of Catalysis, 2001, 197, 229-231.	3.1	582
77	The importance of surface morphology in controlling the selectivity of polycrystalline copper for CO2 electroreduction. Physical Chemistry Chemical Physics, 2012, 14, 76-81.	1.3	576
78	One-Dimensional Metallic Edge States inMoS2. Physical Review Letters, 2001, 87, 196803.	2.9	563
79	First principles calculations and experimental insight into methane steam reforming over transition metal catalysts. Journal of Catalysis, 2008, 259, 147-160.	3.1	559
80	Electrochemical generation of sulfur vacancies in the basal plane of MoS2 for hydrogen evolution. Nature Communications, 2017, 8, 15113.	5.8	555
81	Electrochemical Activation of CO₂ through Atomic Ordering Transformations of AuCu Nanoparticles. Journal of the American Chemical Society, 2017, 139, 8329-8336.	6.6	529
82	Highly selective oxygen reduction to hydrogen peroxide on transition metal single atom coordination. Nature Communications, 2019, 10, 3997.	5.8	528
83	Understanding trends in electrochemical carbon dioxide reduction rates. Nature Communications, 2017, 8, 15438.	5.8	527
84	Ligand effects in heterogeneous catalysis and electrochemistry. Electrochimica Acta, 2007, 52, 5512-5516.	2.6	513
85	Direct and continuous strain control of catalysts with tunable battery electrode materials. Science, 2016, 354, 1031-1036.	6.0	512
86	Electrical conductivity in Li2O2 and its role in determining capacity limitations in non-aqueous Li-O2 batteries. Journal of Chemical Physics, 2011, 135, 214704.	1.2	502
87	The oxygen reduction reaction mechanism on Pt(111) from density functional theory calculations. Electrochimica Acta, 2010, 55, 7975-7981.	2.6	491
88	Surface Pourbaix diagrams and oxygen reduction activity of Pt, Ag and Ni(111) surfaces studied by DFT. Physical Chemistry Chemical Physics, 2008, 10, 3722.	1.3	480
89	Oxygen chemisorption on metal surfaces: General trends for Cu, Ni and Ag. Progress in Surface Science, 1993, 44, 5-66.	3.8	457
90	Universality in Oxygen Reduction Electrocatalysis on Metal Surfaces. ACS Catalysis, 2012, 2, 1654-1660.	5.5	456

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91	Effective-medium theory of chemical binding: Application to chemisorption. Physical Review B, 1980, 21, 2131-2136.	1.1	455
92	Ligand and ensemble effects in adsorption on alloy surfaces. Physical Chemistry Chemical Physics, 2001, 3, 3814-3818.	1.3	455
93	Structure sensitivity in adsorption: CO interaction with stepped and reconstructed Pt surfaces. Catalysis Letters, 1997, 46, 31-35.	1.4	453
94	Structure effects on the energetics of the electrochemical reduction of CO2 by copper surfaces. Surface Science, 2011, 605, 1354-1359.	0.8	445
95	Covalent effects in the effective-medium theory of chemical binding: Hydrogen heats of solution in the3dmetals. Physical Review B, 1982, 26, 2875-2885.	1.1	433
96	Location and coordination of promoter atoms in Co- and Ni-promoted MoS2-based hydrotreating catalysts. Journal of Catalysis, 2007, 249, 220-233.	3.1	428
97	Active edge sites in MoSe₂ and WSe₂ catalysts for the hydrogen evolution reaction: a density functional study. Physical Chemistry Chemical Physics, 2014, 16, 13156-13164.	1.3	426
98	The Mechanism of CO and CO₂ Hydrogenation to Methanol over Cuâ€Based Catalysts. ChemCatChem, 2015, 7, 1105-1111.	1.8	424
99	Quantized conductance in an atom-sized point contact. Physical Review Letters, 1994, 72, 2251-2254.	2.9	414
100	Structure sensitivity of the methanation reaction: H2-induced CO dissociation on nickel surfaces. Journal of Catalysis, 2008, 255, 6-19.	3.1	411
101	Electric Field Effects in Electrochemical CO₂ Reduction. ACS Catalysis, 2016, 6, 7133-7139.	5.5	411
102	Toward Efficient Hydrogen Production at Surfaces. Science, 2006, 312, 1322-1323.	6.0	407
103	Insights into the reactivity of supported Au nanoparticles: combining theory and experiments. Topics in Catalysis, 2007, 44, 15-26.	1.3	402
104	Hydrogen adsorption on metal surfaces. Surface Science, 1984, 136, 59-81.	0.8	400
105	To address surface reaction network complexity using scaling relations machine learning and DFT calculations. Nature Communications, 2017, 8, 14621.	5.8	399
106	A benchmark database for adsorption bond energies to transition metal surfaces and comparison to selected DFT functionals. Surface Science, 2015, 640, 36-44.	0.8	396
107	DFT Calculations of Unpromoted and Promoted MoS2-Based Hydrodesulfurization Catalysts. Journal of Catalysis, 1999, 187, 109-122.	3.1	393
108	Phase diagrams for surface alloys. Physical Review B, 1997, 56, 5822-5834.	1.1	391

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109	Calculated Phase Diagrams for the Electrochemical Oxidation and Reduction of Water over Pt(111). Journal of Physical Chemistry B, 2006, 110, 21833-21839.	1.2	388
110	Effects of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>d</mml:mi></mml:math>-band shape on the surface reactivity of transition-metal alloys. Physical Review B, 2014, 89, .	1.1	387
111	Understanding trends in Câ€“H bond activation in heterogeneous catalysis. Nature Materials, 2017, 16, 225-229.	13.3	387
112	Dependence of the He-Scattering Potential at Surfaces on the Surface-Electron-Density Profile. Physical Review Letters, 1980, 45, 807-810.	2.9	386
113	CO Oxidation on Rutile-Supported Au Nanoparticles. Angewandte Chemie - International Edition, 2005, 44, 1824-1826.	7.2	381
114	Trends in the Catalytic CO Oxidation Activity of Nanoparticles. Angewandte Chemie - International Edition, 2008, 47, 4835-4839.	7.2	381
115	Atomic-scale insight into structure and morphology changes of MoS2 nanoclusters in hydrotreating catalysts. Journal of Catalysis, 2004, 221, 510-522.	3.1	379
116	Trends in electrochemical CO2 reduction activity for open and close-packed metal surfaces. Physical Chemistry Chemical Physics, 2014, 16, 4720.	1.3	375
117	Towards an ammonia-mediated hydrogen economy?. Catalysis Today, 2006, 111, 140-144.	2.2	372
118	Electrostatic adsorbate-adsorbate interactions: The poisoning and promotion of the molecular adsorption reaction. Surface Science, 1985, 150, 24-38.	0.8	371
119	pH effects on the electrochemical reduction of CO(2) towards C2 products on stepped copper. Nature Communications, 2019, 10, 32.	5.8	371
120	Secondary-ion emission probability in sputtering. Physical Review B, 1979, 19, 5661-5665.	1.1	370
121	Exploring the limits: A low-pressure, low-temperature Haberâ€“Bosch process. Chemical Physics Letters, 2014, 598, 108-112.	1.2	369
122	Bonding of Gold Nanoclusters to Oxygen Vacancies on RutileTiO2(110). Physical Review Letters, 2003, 90, 026101.	2.9	367
123	Communications: Elementary oxygen electrode reactions in the aprotic Li-air battery. Journal of Chemical Physics, 2010, 132, 071101.	1.2	367
124	Universal transition state scaling relations for (de)hydrogenation over transition metals. Physical Chemistry Chemical Physics, 2011, 13, 20760.	1.3	363
125	Atomic and electronic structure ofMoS2nanoparticles. Physical Review B, 2003, 67, .	1.1	352
126	Hydrogen Evolution Over Bimetallic Systems: Understanding the Trends. ChemPhysChem, 2006, 7, 1032-1035.	1.0	351

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127	The electronic structure effect in heterogeneous catalysis. Catalysis Letters, 2005, 100, 111-114.	1.4	349
128	Modeling the electrified solidâ€“liquid interface. Chemical Physics Letters, 2008, 466, 68-71.	1.2	349
129	Optimizing Perovskites for the Water-Splitting Reaction. Science, 2011, 334, 1355-1356.	6.0	349
130	Ammonia synthesis from N₂and H₂O using a lithium cycling electrification strategy at atmospheric pressure. Energy and Environmental Science, 2017, 10, 1621-1630.	15.6	342
131	Insights into Cï£¿C Coupling in CO₂ Electroreduction on Copper Electrodes. ChemCatChem, 2013, 5, 737-742.	1.8	339
132	Unifying Kinetic and Thermodynamic Analysis of 2 e^{â€“} and 4 e^{â€“} Reduction of Oxygen on Metal Surfaces. Journal of Physical Chemistry C, 2014, 118, 6706-6718.	1.5	337
133	Multidimensional Potential Energy Surface forH2Dissociation over Cu(111). Physical Review Letters, 1994, 73, 1400-1403.	2.9	334
134	Understanding activity trends in electrochemical water oxidation to form hydrogen peroxide. Nature Communications, 2017, 8, 701.	5.8	333
135	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.	1.3	332
136	Anode Materials for Low-Temperature Fuel Cells: A Density Functional Theory Study. Journal of Catalysis, 2001, 199, 123-131.	3.1	330
137	CatMAP: A Software Package for Descriptor-Based Microkinetic Mapping of Catalytic Trends. Catalysis Letters, 2015, 145, 794-807.	1.4	328
138	Electrochemical dissolution of surface alloys in acids: Thermodynamic trends from first-principles calculations. Electrochimica Acta, 2007, 52, 5829-5836.	2.6	326
139	Transition-Metal Single Atoms in a Graphene Shell as Active Centers for Highly Efficient Artificial Photosynthesis. CheM, 2017, 3, 950-960.	5.8	326
140	Initial growth of Au on Ni(110): Surface alloying of immiscible metals. Physical Review Letters, 1993, 71, 754-757.	2.9	325
141	Direct observation of the oxygenated species during oxygen reduction on a platinum fuel cell cathode. Nature Communications, 2013, 4, .	5.8	325
142	Microscopic model for the poisoning and promotion of adsorption rates by electronegative and electropositive atoms. Surface Science, 1984, 137, 65-78.	0.8	320
143	Assessing the reliability of calculated catalytic ammonia synthesis rates. Science, 2014, 345, 197-200.	6.0	319
144	Theoretical insights into the hydrogen evolution activity of layered transition metal dichalcogenides. Surface Science, 2015, 640, 133-140.	0.8	315

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145	Toward computational screening in heterogeneous catalysis: Pareto-optimal methanation catalysts. Journal of Catalysis, 2006, 239, 501-506.	3.1	314
146	Chemisorption on metal surfaces. Reports on Progress in Physics, 1990, 53, 1253-1295.	8.1	313
147	Theoretical Insight into the Trends that Guide the Electrochemical Reduction of Carbon Dioxide to Formic Acid. ChemSusChem, 2016, 9, 358-363.	3.6	311
148	Designing Boron Nitride Islands in Carbon Materials for Efficient Electrochemical Synthesis of Hydrogen Peroxide. Journal of the American Chemical Society, 2018, 140, 7851-7859.	6.6	310
149	Electrochemical Barriers Made Simple. Journal of Physical Chemistry Letters, 2015, 6, 2663-2668.	2.1	309
150	Hydrodesulfurization reaction pathways on MoS2 nanoclusters revealed by scanning tunneling microscopy. Journal of Catalysis, 2004, 224, 94-106.	3.1	308
151	Quantized conductance in atom-sized wires between two metals. Physical Review B, 1995, 52, 8499-8514.	1.1	307
152	Importance of Correlation in Determining Electrocatalytic Oxygen Evolution Activity on Cobalt Oxides. Journal of Physical Chemistry C, 2012, 116, 21077-21082.	1.5	305
153	Electrochemical Carbon Monoxide Reduction on Polycrystalline Copper: Effects of Potential, Pressure, and pH on Selectivity toward Multicarbon and Oxygenated Products. ACS Catalysis, 2018, 8, 7445-7454.	5.5	305
154	Trends in the chemical properties of early transition metal carbide surfaces: A density functional study. Catalysis Today, 2005, 105, 66-73.	2.2	302
155	Scaling Relationships for Adsorption Energies on Transition Metal Oxide, Sulfide, and Nitride Surfaces. Angewandte Chemie - International Edition, 2008, 47, 4683-4686.	7.2	301
156	Machine-Learning Methods Enable Exhaustive Searches for Active Bimetallic Facets and Reveal Active Site Motifs for CO₂ Reduction. ACS Catalysis, 2017, 7, 6600-6608.	5.5	300
157	Bridging the "Pressure Gap" between Ultrahigh-Vacuum Surface Physics and High-Pressure Catalysis. Physical Review Letters, 1985, 55, 2502-2505.	2.9	288
158	Modeling the electro-oxidation of CO and H2/CO on Pt, Ru, PtRu and Pt3Sn. Electrochimica Acta, 2003, 48, 3731-3742.	2.6	285
159	New design paradigm for heterogeneous catalysts. National Science Review, 2015, 2, 140-143.	4.6	280
160	Unifying the 2e^{â€“} and 4e^{â€“} Reduction of Oxygen on Metal Surfaces. Journal of Physical Chemistry Letters, 2012, 3, 2948-2951.	2.1	276
161	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
162	Effect of strain on surface diffusion and nucleation. Physical Review B, 1995, 52, R14380-R14383.	1.1	274

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163	Recent STM, DFT and HAADF-STEM studies of sulfide-based hydrotreating catalysts: Insight into mechanistic, structural and particle size effects. Catalysis Today, 2008, 130, 86-96.	2.2	265
164	Universal BrÃ¸nsted-Evans-Polanyi Relations for Câ€“C, Câ€“O, Câ€“N, Nâ€“O, Nâ€“N, and Oâ€“O Dissociation Reactions. Catalysis Letters, 2011, 141, 370-373.	1.4	265
165	Sintering of nickel steam-reforming catalysts: effects of temperature and steam and hydrogen pressures. Journal of Catalysis, 2004, 223, 432-443.	3.1	264
166	Controlling the catalytic bond-breaking selectivity of Ni surfaces by step blocking. Nature Materials, 2005, 4, 160-162.	13.3	263
167	A theoretical study of CH4 dissociation on pure and goldâ€alloyed Ni(111) surfaces. Journal of Chemical Physics, 1996, 105, 5595-5604.	1.2	262
168	Estimations of electric field effects on the oxygen reduction reaction based on the density functional theory. Physical Chemistry Chemical Physics, 2007, 9, 5158.	1.3	260
169	Ammonia synthesis over a Ru(0001) surface studied by density functional calculations. Journal of Catalysis, 2003, 220, 273-279.	3.1	259
170	How a gold substrate can increase the reactivity of a Pt overlayer. Surface Science, 1999, 426, 395-409.	0.8	258
171	Molybdenum Sulfides and Selenides as Possible Electrocatalysts for CO₂ Reduction. ChemCatChem, 2014, 6, 1899-1905.	1.8	255
172	Kinetic Implications of Dynamical Changes in Catalyst Morphology during Methanol Synthesis over Cu/ZnO Catalysts. Journal of Catalysis, 1997, 168, 133-142.	3.1	254
173	How Doped MoS₂ Breaks Transition-Metal Scaling Relations for CO₂ Electrochemical Reduction. ACS Catalysis, 2016, 6, 4428-4437.	5.5	254
174	The hydrogenation and direct desulfurization reaction pathway in thiophene hydrodesulfurization over MoS2 catalysts at realistic conditions: A density functional study. Journal of Catalysis, 2007, 248, 188-203.	3.1	253
175	Investigation of Catalytic Finite-Size-Effects of Platinum Metal Clusters. Journal of Physical Chemistry Letters, 2013, 4, 222-226.	2.1	249
176	Combined Electronic Structure and Evolutionary Search Approach to Materials Design. Physical Review Letters, 2002, 88, 255506.	2.9	248
177	Mechanisms for catalytic carbon nanofiber growth studied byab initiodensity functional theory calculations. Physical Review B, 2006, 73, .	1.1	248
178	A kinetic model of the water gas shift reaction. Journal of Catalysis, 1992, 134, 445-468.	3.1	244
179	Trends in CO Oxidation Rates for Metal Nanoparticles and Close-Packed, Stepped, and Kinked Surfaces. Journal of Physical Chemistry C, 2009, 113, 10548-10553.	1.5	244
180	The adhesion and shape of nanosized Au particles in a Au/TiO2 catalyst. Journal of Catalysis, 2004, 225, 86-94.	3.1	240

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181	A Kinetic Model of Methanol Synthesis. Journal of Catalysis, 1995, 156, 229-242.	3.1	239
182	Electronic Structure Effects in Transition Metal Surface Chemistry. Topics in Catalysis, 2014, 57, 25-32.	1.3	238
183	Defective Carbon-Based Materials for the Electrochemical Synthesis of Hydrogen Peroxide. ACS Sustainable Chemistry and Engineering, 2018, 6, 311-317.	3.2	236
184	Finite Size Effects in Chemical Bonding: From Small Clusters to Solids. Catalysis Letters, 2011, 141, 1067-1071.	1.4	234
185	One- or Two-Electron Water Oxidation, Hydroxyl Radical, or H₂O₂ Evolution. Journal of Physical Chemistry Letters, 2017, 8, 1157-1160.	2.1	234
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