Frank Abild-Pedersen

List of Publications by Year
in descending order

158 papers	33,878 citations	13087 68 h-index	4988 167 g-index
182 all docs	182 docs citations	182 times ranked	26753 citing authors

#	Article	IF	Citations
1	How copper catalyzes the electroreduction of carbon dioxide into hydrocarbon fuels. Energy and Environmental Science, 2010, 3, 1311.	15.6	2,682
2	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
3	The Active Site of Methanol Synthesis over Cu/ZnO/Al ₂ O ₃ Industrial Catalysts. Science, 2012, 336, 893-897.	6.0	2,018
4	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
5	Atomic-scale imaging of carbon nanofibre growth. Nature, 2004, 427, 426-429.	13.7	1,318
6	From the Sabatier principle to a predictive theory of transition-metal heterogeneous catalysis. Journal of Catalysis, 2015, 328, 36-42.	3.1	1,271
7	Scaling Properties of Adsorption Energies for Hydrogen-Containing Molecules on Transition-Metal Surfaces. Physical Review Letters, 2007, 99, 016105.	2.9	1,270
8	A theoretical evaluation of possible transition metal electro-catalysts for N₂reduction. Physical Chemistry Chemical Physics, 2012, 14, 1235-1245.	1.3	1,184
9	Identification of Non-Precious Metal Alloy Catalysts for Selective Hydrogenation of Acetylene. Science, 2008, 320, 1320-1322.	6.0	984
10	Discovery of a Ni-Ga catalyst for carbon dioxide reduction to methanol. Nature Chemistry, 2014, 6, 320-324.	6.6	865
11	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
12	The nature of the active site in heterogeneous metal catalysis. Chemical Society Reviews, 2008, 37, 2163.	18.7	703
13	Tuning the MoS₂ Edge-Site Activity for Hydrogen Evolution via Support Interactions. Nano Letters, 2014, 14, 1381-1387.	4.5	660
14	Transition-metal doped edge sites in vertically aligned MoS2 catalysts for enhanced hydrogen evolution. Nano Research, 2015, 8, 566-575.	5.8	594
15	First principles calculations and experimental insight into methane steam reforming over transition metal catalysts. Journal of Catalysis, 2008, 259, 147-160.	3.1	559
16	Electrochemical generation of sulfur vacancies in the basal plane of MoS2 for hydrogen evolution. Nature Communications, 2017, 8, 15113.	5.8	555
17	Direct and continuous strain control of catalysts with tunable battery electrode materials. Science, 2016, 354, 1031-1036.	6.0	512
18	Enhancing Electrocatalytic Water Splitting by Strain Engineering. Advanced Materials, 2019, 31, e1807001.	11.1	470

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19	Structure effects on the energetics of the electrochemical reduction of CO2 by copper surfaces. Surface Science, 2011, 605, 1354-1359.	0.8	445
20	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
21	The Mechanism of CO and CO₂ Hydrogenation to Methanol over Cuâ€Based Catalysts. ChemCatChem, 2015, 7, 1105-1111.	1.8	424
22	Structure sensitivity of the methanation reaction: H2-induced CO dissociation on nickel surfaces. Journal of Catalysis, 2008, 255, 6-19.	3.1	411
23	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
24	Understanding trends in Câ€“H bond activation in heterogeneous catalysis. Nature Materials, 2017, 16, 225-229.	13.3	387
25	Exploring the limits: A low-pressure, low-temperature Haberâ€“Bosch process. Chemical Physics Letters, 2014, 598, 108-112.	1.2	369
26	Universal transition state scaling relations for (de)hydrogenation over transition metals. Physical Chemistry Chemical Physics, 2011, 13, 20760.	1.3	363
27	Assessing the reliability of calculated catalytic ammonia synthesis rates. Science, 2014, 345, 197-200.	6.0	319
28	Electrochemical chlorine evolution at rutile oxide (110) surfaces. Physical Chemistry Chemical Physics, 2010, 12, 283-290.	1.3	317
29	Theoretical insights into the hydrogen evolution activity of layered transition metal dichalcogenides. Surface Science, 2015, 640, 133-140.	0.8	315
30	Scaling Relationships for Adsorption Energies on Transition Metal Oxide, Sulfide, and Nitride Surfaces. Angewandte Chemie - International Edition, 2008, 47, 4683-4686.	7.2	301
31	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
32	CO adsorption energies on metals with correction for high coordination adsorption sites â€“ A density functional study. Surface Science, 2007, 601, 1747-1753.	0.8	259
33	Hydrogenation of CO2 to methanol and CO on Cu/ZnO/Al2O3: Is there a common intermediate or not?. Journal of Catalysis, 2015, 328, 43-48.	3.1	252
34	Investigation of Catalytic Finite-Size-Effects of Platinum Metal Clusters. Journal of Physical Chemistry Letters, 2013, 4, 222-226.	2.1	249
35	Mechanisms for catalytic carbon nanofiber growth studied byab initiodensity functional theory calculations. Physical Review B, 2006, 73, .	1.1	248
36	Electronic Structure Effects in Transition Metal Surface Chemistry. Topics in Catalysis, 2014, 57, 25-32.	1.3	238

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37	Dynamical Observation and Detailed Description of Catalysts under Strong Metalâ€“Support Interaction. Nano Letters, 2016, 16, 4528-4534.	4.5	230
38	Methane activation on Ni(111): Effects of poisons and step defects. Surface Science, 2005, 590, 127-137.	0.8	228
39	On the Role of Surface Modifications of Palladium Catalysts in the Selective Hydrogenation of Acetylene. Angewandte Chemie - International Edition, 2008, 47, 9299-9302.	7.2	222
40	Machine Learning for Computational Heterogeneous Catalysis. ChemCatChem, 2019, 11, 3581-3601.	1.8	220
41	On the effect of coverage-dependent adsorbateâ€“adsorbate interactions for CO methanation on transition metal surfaces. Journal of Catalysis, 2013, 307, 275-282.	3.1	217
42	Theoretical Analysis of Transition-Metal Catalysts for Formic Acid Decomposition. ACS Catalysis, 2014, 4, 1226-1233.	5.5	209
43	CO hydrogenation to methanol on Cuâ€“Ni catalysts: Theory and experiment. Journal of Catalysis, 2012, 293, 51-60.	3.1	195
44	Probing the transition state region in catalytic CO oxidation on Ru. Science, 2015, 347, 978-982.	6.0	193
45	Activity and Selectivity Trends in Synthesis Gas Conversion to Higher Alcohols. Topics in Catalysis, 2014, 57, 135-142.	1.3	173
46	Revealing the Synergy between Oxide and Alloy Phases on the Performance of Bimetallic Inâ€“Pd Catalysts for CO₂ Hydrogenation to Methanol. ACS Catalysis, 2019, 9, 3399-3412.	5.5	173
47	Catalyst deactivation via decomposition into single atoms and the role of metal loading. Nature Catalysis, 2019, 2, 748-755.	16.1	171
48	Rational design of MoS₂ catalysts: tuning the structure and activity via transition metal doping. Catalysis Science and Technology, 2015, 5, 246-253.	2.1	152
49	Systematic Structureâ€“Property Relationship Studies in Palladium-Catalyzed Methane Complete Combustion. ACS Catalysis, 2017, 7, 7810-7821.	5.5	151
50	CO and CO2 Hydrogenation to Methanol Calculated Using the BEEF-vdW Functional. Catalysis Letters, 2013, 143, 71-73.	1.4	148
51	On the behavior of BrÃ¸nsted-Evans-Polanyi relations for transition metal oxides. Journal of Chemical Physics, 2011, 134, 244509.	1.2	128
52	CatApp: A Web Application for Surface Chemistry and Heterogeneous Catalysis. Angewandte Chemie - International Edition, 2012, 51, 272-274.	7.2	126
53	On the Role of Metal Step-Edges in Graphene Growth. Journal of Physical Chemistry C, 2010, 114, 11221-11227.	1.5	110
54	Interlayer Carbon Bond Formation Induced by Hydrogen Adsorption in Few-Layer Supported Graphene. Physical Review Letters, 2013, 111, 085503.	2.9	110

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55	Chemical and Phase Evolution of Amorphous Molybdenum Sulfide Catalysts for Electrochemical Hydrogen Production. ACS Nano, 2016, 10, 624-632.	7.3	109
56	Scaling relationships for adsorption energies of C2 hydrocarbons on transition metal surfaces. Chemical Engineering Science, 2011, 66, 6318-6323.	1.9	108
57	DFT Study of Formaldehyde and Methanol Synthesis from CO and H2on Ni(111)â€. Journal of Physical Chemistry B, 2004, 108, 14535-14540.	1.2	102
58	Elementary steps of syngas reactions on Mo2C(001): Adsorption thermochemistry and bond dissociation. Journal of Catalysis, 2012, 290, 108-117.	3.1	96
59	Using scaling relations to understand trends in the catalytic activity of transition metals. Journal of Physics Condensed Matter, 2008, 20, 064239.	0.7	92
60	Mechanistic insights into heterogeneous methane activation. Physical Chemistry Chemical Physics, 2017, 19, 3575-3581.	1.3	89
61	Electronic Origin of the Surface Reactivity of Transition-Metal-Doped TiO₂(110). Journal of Physical Chemistry C, 2013, 117, 460-465.	1.5	87
62	Operando Characterization of an Amorphous Molybdenum Sulfide Nanoparticle Catalyst during the Hydrogen Evolution Reaction. Journal of Physical Chemistry C, 2014, 118, 29252-29259.	1.5	87
63	From electricity to fuels: Descriptors for C1 selectivity in electrochemical CO2 reduction. Applied Catalysis B: Environmental, 2020, 279, 119384.	10.8	81
64	Descriptorâ€Based Analysis Applied to HCN Synthesis from NH₃ and CH₄. Angewandte Chemie - International Edition, 2011, 50, 4601-4605.	7.2	80
65	Investigating Catalystâ€“Support Interactions To Improve the Hydrogen Evolution Reaction Activity of Thiomolybdate [Mo₃S₁₃]^{2â€“} Nanoclusters. ACS Catalysis, 2017, 7, 7126-7130.	5.5	76
66	Understanding the Effect of Steps, Strain, Poisons, and Alloying: Methane Activation on Ni Surfaces. Catalysis Letters, 2005, 105, 9-13.	1.4	74
67	Sintering of Pt Nanoparticles via Volatile PtO₂: Simulation and Comparison with Experiments. ACS Catalysis, 2016, 6, 7098-7108.	5.5	72
68	Mechanistic Insights into the Synthesis of Higher Alcohols from Syngas on CuCo Alloys. ACS Catalysis, 2018, 8, 10148-10155.	5.5	71
69	Understanding the Reactivity of Layered Transition-Metal Sulfides: A Single Electronic Descriptor for Structure and Adsorption. Journal of Physical Chemistry Letters, 2014, 5, 3884-3889.	2.1	70
70	A Highly Active Molybdenum Phosphide Catalyst for Methanol Synthesis from CO and CO₂. Angewandte Chemie - International Edition, 2018, 57, 15045-15050.	7.2	69
71	BrÃ¸nstedâ€“Evansâ€“Polanyi Relationship for Transition Metal Carbide and Transition Metal Oxide Surfaces. Journal of Physical Chemistry C, 2013, 117, 4168-4171.	1.5	67
72	Rh-MnO Interface Sites Formed by Atomic Layer Deposition Promote Syngas Conversion to Higher Oxygenates. ACS Catalysis, 2017, 7, 5746-5757.	5.5	66

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73	Selectivity of Synthesis Gas Conversion to C₂₊ Oxygenates on fcc(111) Transition-Metal Surfaces. ACS Catalysis, 2018, 8, 3447-3453.	5.5	66
74	In silicosearch for novel methane steam reforming catalysts. New Journal of Physics, 2013, 15, 125021.	1.2	65
75	Energetics of Oxygen Adatoms, Hydroxyl Species and Water Dissociation on Pt(111). Journal of Physical Chemistry C, 2012, 116, 25772-25776.	1.5	62
76	The role of atomic carbon in directing electrochemical CO₍₂₎ reduction to multicarbon products. Energy and Environmental Science, 2021, 14, 473-482.	15.6	62
77	Surface Tension Effects on the Reactivity of Metal Nanoparticles. Journal of Physical Chemistry Letters, 2015, 6, 3797-3801.	2.1	59
78	Two-Dimensional Materials as Catalysts for Energy Conversion. Catalysis Letters, 2016, 146, 1917-1921.	1.4	58
79	Structureâ€Sensitive Scaling Relations: Adsorption Energies from Surface Site Stability. ChemCatChem, 2018, 10, 1643-1650.	1.8	57
80	Trends in oxygenate/hydrocarbon selectivity for electrochemical CO(2) reduction to C2 products. Nature Communications, 2022, 13, 1399.	5.8	56
81	On the role of the surface oxygen species during Aâ€“H (A = C, N, O) bond activation: a density functional theory study. Chemical Communications, 2015, 51, 2621-2624.	2.2	51
82	Volcano Relation for the Deacon Process over Transitionâ€Metal Oxides. ChemCatChem, 2010, 2, 98-102.	1.8	49
83	Computational catalyst screening: Scaling, bond-order and catalysis. Catalysis Today, 2016, 272, 6-13.	2.2	48
84	Insights into carbon nanotube nucleation: Cap formation governed by catalyst interfacial step flow. Scientific Reports, 2014, 4, 6510.	1.6	46
85	Catalysis in real time using X-ray lasers. Chemical Physics Letters, 2017, 675, 145-173.	1.2	45
86	Enhancing the connection between computation and experiments in electrocatalysis. Nature Catalysis, 2022, 5, 374-381.	16.1	45
87	Self Blocking of CO Dissociation on a Stepped Ruthenium Surface. Topics in Catalysis, 2010, 53, 357-364.	1.3	44
88	Metal Oxideâ€Supported Platinum Overlayers as Protonâ€Exchange Membrane Fuel Cell Cathodes. ChemCatChem, 2012, 4, 228-235.	1.8	44
89	Nature of Lone-Pairâ€“Surface Bonds and Their Scaling Relations. Inorganic Chemistry, 2018, 57, 7222-7238.	1.9	43
90	Bimetallic effects on Zn-Cu electrocatalysts enhance activity and selectivity for the conversion of CO2 to CO. Chem Catalysis, 2021, 1, 663-680.	2.9	42

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91	Application of a new informatics tool in heterogeneous catalysis: Analysis of methanol dehydrogenation on transition metal catalysts for the production of anhydrous formaldehyde. Journal of Catalysis, 2012, 291, 133-137.	3.1	41
92	Understanding Structureâ€“Property Relationships of MoO₃-Promoted Rh Catalysts for Syngas Conversion to Alcohols. Journal of the American Chemical Society, 2019, 141, 19655-19668.	6.6	41
93	Predicting Adsorption Properties of Catalytic Descriptors on Bimetallic Nanoalloys with Site-Specific Precision. Journal of Physical Chemistry Letters, 2019, 10, 1852-1859.	2.1	41
94	Configurational Energies of Nanoparticles Based on Metalâ€“Metal Coordination. Journal of Physical Chemistry C, 2017, 121, 23002-23010.	1.5	40
95	Theoretical Insights into Methane Câ€“H Bond Activation on Alkaline Metal Oxides. Journal of Physical Chemistry C, 2017, 121, 16440-16446.	1.5	40
96	First-principles investigations of the Ni3Sn alloy at steam reforming conditions. Surface Science, 2009, 603, 762-770.	0.8	39
97	Scaling Relations for Adsorption Energies on Doped Molybdenum Phosphide Surfaces. ACS Catalysis, 2017, 7, 2528-2534.	5.5	39
98	The Role of Roughening to Enhance Selectivity to C₂₊ Products during CO₂ Electroreduction on Copper. ACS Energy Letters, 2021, 6, 3252-3260.	8.8	38
99	Theoretical Investigation of Methane Oxidation on Pd(111) and Other Metallic Surfaces. Journal of Physical Chemistry C, 2018, 122, 16023-16032.	1.5	34
100	A coordination-based model for transition metal alloy nanoparticles. Nanoscale, 2019, 11, 4438-4452.	2.8	34
101	Achieving industrial ammonia synthesis rates at near-ambient conditions through modified scaling relations on a confined dual site. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	34
102	Catalytic Performance and Near-Surface X-ray Characterization of Titanium Hydride Electrodes for the Electrochemical Nitrate Reduction Reaction. Journal of the American Chemical Society, 2022, 144, 5739-5744.	6.6	31
103	Bond control in surface reactions. Nature, 2009, 461, 1223-1225.	13.7	29
104	An orbital-overlap model for minimal work functions of cesiated metal surfaces. Journal of Physics Condensed Matter, 2012, 24, 445007.	0.7	29
105	Energetics of the Waterâ€“Gas-Shift Reaction on the Active Sites of the Industrially Used Cu/ZnO/Al2O3 Catalyst. Catalysis Letters, 2014, 144, 1973-1977.	1.4	29
106	Modeling the Migration of Platinum Nanoparticles on Surfaces Using a Kinetic Monte Carlo Approach. Journal of Physical Chemistry C, 2017, 121, 4261-4269.	1.5	29
107	Reversible graphene-metal contact through hydrogenation. Physical Review B, 2012, 86, .	1.1	28
108	Strong Influence of Coadsorbate Interaction on CO Desorption Dynamics on Ru(0001) Probed by Ultrafast X-Ray Spectroscopy andAbÂInitioSimulations. Physical Review Letters, 2015, 114, 156101.	2.9	25

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109	Bond Order Conservation Strategies in Catalysis Applied to the NH₃ Decomposition Reaction. ACS Catalysis, 2017, 7, 864-871.	5.5	25
110	Modeling Potential-Dependent Electrochemical Activation Barriers: Revisiting the Alkaline Hydrogen Evolution Reaction. Journal of the American Chemical Society, 2021, 143, 19341-19355.	6.6	25
111	Insights and comparison of structureâ€“property relationships in propane and propene catalytic combustion on Pd- and Pt-based catalysts. Journal of Catalysis, 2021, 401, 89-101.	3.1	24
112	Colloidal Platinumâ€“Copper Nanocrystal Alloy Catalysts Surpass Platinum in Low-Temperature Propene Combustion. Journal of the American Chemical Society, 2022, 144, 1612-1621.	6.6	24
113	Elucidating the electronic structure of supported gold nanoparticles and its relevance to catalysis by means of hard X-ray photoelectron spectroscopy. Surface Science, 2016, 650, 24-33.	0.8	23
114	Spin Uncoupling in Chemisorbed OCCO and CO₂: Two High-Energy Intermediates in Catalytic CO₂ Reduction. Journal of Physical Chemistry C, 2018, 122, 12251-12258.	1.5	22
115	Examining the Linearity of Transition State Scaling Relations. Journal of Physical Chemistry C, 2015, 119, 10448-10453.	1.5	21
116	Chemical Bond Activation Observed with an X-ray Laser. Journal of Physical Chemistry Letters, 2016, 7, 3647-3651.	2.1	21
117	Theory-Aided Discovery of Metallic Catalysts for Selective Propane Dehydrogenation to Propylene. ACS Catalysis, 2021, 11, 6290-6297.	5.5	21
118	Inherent Enhancement of Electronic Emission from Hexaboride Heterostructure. Physical Review Applied, 2014, 2, .	1.5	20
119	Trends in the Thermodynamic Stability of Ultrathin Supported Oxide Films. Journal of Physical Chemistry C, 2016, 120, 10351-10360.	1.5	19
120	Engineering high-performance Pd coreâ€“MgO porous shell nanocatalysts via heterogeneous gas-phase synthesis. Nanoscale, 2015, 7, 13387-13392.	2.8	18
121	Modeling the Interface of Platinum and Î±-Quartz(001): Implications for Sintering. Journal of Physical Chemistry C, 2016, 120, 10340-10350.	1.5	18
122	Exploring Trends on Coupling Mechanisms toward C₃ Product Formation in CO₍₂₎R. Journal of Physical Chemistry C, 2021, 125, 26437-26447.	1.5	18
123	Theoretical and Experimental Studies of CoGa Catalysts for the Hydrogenation of CO2 to Methanol. Catalysis Letters, 2018, 148, 3583-3591.	1.4	17
124	Enhanced CO tolerance of Pt clusters supported on graphene with lattice vacancies. Physical Review B, 2020, 102, .	1.1	17
125	Trends for Methane Oxidation at Solid Oxide Fuel Cell Conditions. Journal of the Electrochemical Society, 2009, 156, B1447.	1.3	16
126	Tuning Methane Activation Chemistry on Alkaline Earth Metal Oxides by Doping. Journal of Physical Chemistry C, 2018, 122, 22544-22548.	1.5	16

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127	Low-Temperature Methane Partial Oxidation to Syngas with Modular Nanocrystal Catalysts. ACS Applied Nano Materials, 2018, 1, 5258-5267.	2.4	16
128	Revealing the structure of a catalytic combustion active-site ensemble combining uniform nanocrystal catalysts and theory insights. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 14721-14729.	3.3	16
129	Guiding the Catalytic Properties of Copper for Electrochemical CO₂ Reduction by Metal Atom Decoration. ACS Applied Materials & Interfaces, 2021, 13, 52044-52054.	4.0	16
130	Comment on â€œUsing Photoelectron Spectroscopy and Quantum Mechanics to Determine d-Band Energies of Metals for Catalytic Applicationsâ€• Journal of Physical Chemistry C, 2013, 117, 6914-6915.	1.5	15
131	A Highly Active Molybdenum Phosphide Catalyst for Methanol Synthesis from CO and CO₂. Angewandte Chemie, 2018, 130, 15265-15270.	1.6	15
132	DFT Study of Atomically-Modified Alkali-Earth Metal Oxide Films on Tungsten. Journal of Physical Chemistry C, 2014, 118, 11303-11309.	1.5	13
133	Predicting Promoter-Induced Bond Activation on Solid Catalysts Using Elementary Bond Orders. Journal of Physical Chemistry Letters, 2015, 6, 3670-3674.	2.1	13
134	Comparison of Sintering by Particle Migration and Ripening through First-Principles-Based Simulations. Journal of Physical Chemistry C, 2018, 122, 26563-26569.	1.5	13
135	Combining artificial intelligence and physics-based modeling to directly assess atomic site stabilities: from sub-nanometer clusters to extended surfaces. Physical Chemistry Chemical Physics, 2021, 23, 22022-22034.	1.3	13
136	Microkinetic Modeling of Propene Combustion on a Stepped, Metallic Palladium Surface and the Importance of Oxygen Coverage. ACS Catalysis, 2022, 12, 1742-1757.	5.5	13
137	Carbide induced reconstruction of monatomic steps on Ni(111) â€“ A density functional study. Surface Science, 2007, 601, 649-655.	0.8	12
138	Methanol Partial Oxidation on Ag(1â€‰1â€‰1) from First Principles. ChemCatChem, 2016, 8, 3621-3625.	1.8	12
139	Predicting metalâ€“metal interactions. I. The influence of strain on nanoparticle and metal adlayer stabilities. Journal of Chemical Physics, 2020, 152, 094701.	1.2	12
140	First-principles investigations of Ni3Al(111) and NiAl(110) surfaces at metal dusting conditions. Surface Science, 2011, 605, 582-592.	0.8	11
141	Volcano Relations for Oxidation of Hydrogen Halides over Rutile Oxide Surfaces. ChemCatChem, 2012, 4, 1856-1861.	1.8	11
142	Ultrafast Adsorbate Excitation Probed with Subpicosecond-Resolution X-Ray Absorption Spectroscopy. Physical Review Letters, 2021, 127, 016802.	2.9	11
143	Dynamics and Hysteresis of Hydrogen Intercalation and Deintercalation in Palladium Electrodes: A Multimodal In Situ X-ray Diffraction, Coulometry, and Computational Study. Chemistry of Materials, 2021, 33, 5872-5884.	3.2	11
144	Thermionic current densities from first principles. Journal of Chemical Physics, 2013, 138, 204701.	1.2	10

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145	Identification of earth-abundant materials for selective dehydrogenation of light alkanes to olefins. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	10
146	Real-Time Elucidation of Catalytic Pathways in CO Hydrogenation on Ru. Journal of Physical Chemistry Letters, 2017, 8, 3820-3825.	2.1	9
147	Generic approach to access barriers in dehydrogenation reactions. Communications Chemistry, 2018, 1, .	2.0	9
148	Strongly Modified Scaling of CO Hydrogenation in Metal Supported TiO Nanostripes. ACS Catalysis, 2018, 8, 10555-10563.	5.5	8
149	Predicting metalâ€“metal interactions. II. Accelerating generalized schemes through physical insights. Journal of Chemical Physics, 2020, 152, 094702.	1.2	8
150	Identifying factors controlling the selective ethane dehydrogenation on Pt-based catalysts from DFT based micro-kinetic modeling. Journal of Energy Chemistry, 2021, 58, 37-40.	7.1	8
151	Efficient Screening of Biâ€“Metallic Electrocatalysts for Glycerol Valorization. Electrochimica Acta, 2021, 398, 139283.	2.6	8
152	Unraveling Electronic Trends in O* and OH* Surface Adsorption in the MO₂ Transition-Metal Oxide Series. Journal of Physical Chemistry C, 2022, 126, 7903-7909.	1.5	8
153	Analysis of sulfur-induced selectivity changes for anhydrous methanol dehydrogenation on Ni(100) surfaces. Surface Science, 2013, 613, 58-62.	0.8	7
154	Toward Controlled Growth of Helicity-Specific Carbon Nanotubes. Journal of Physical Chemistry Letters, 2015, 6, 2232-2237.	2.1	7
155	A Theoretical Study of Methanol Oxidation on RuO₂(110): Bridging the Pressure Gap. ACS Catalysis, 2017, 7, 4527-4534.	5.5	6
156	Accuracy of XAS theory for unraveling structural changes of adsorbates: CO on Ni(100). AIP Advances, 2020, 10, 115014.	0.6	6
157	Stability of Pt-Modified Cu(111) in the Presence of Oxygen and Its Implication on the Overall Electronic Structure. Journal of Physical Chemistry C, 2013, 117, 16371-16380.	1.5	5
158	Accessing the Câ€“C transition state energy on transition metals. Physical Chemistry Chemical Physics, 2019, 21, 25328-25333.	1.3	3