Felix Studt

List of Publications by Year in descending order

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156 papers	23,903 citations	18436 62 h-index	7718 150 g-index
175 all docs	175 docs citations	175 times ranked	18402 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	The Active Site of Methanol Synthesis over Cu/ZnO/Al ₂ O ₃ Industrial Catalysts. Science, 2012, 336, 893-897.	6.0	2,018
3	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
4	From the Sabatier principle to a predictive theory of transition-metal heterogeneous catalysis. Journal of Catalysis, 2015, 328, 36-42.	3.1	1,271
5	Scaling Properties of Adsorption Energies for Hydrogen-Containing Molecules on Transition-Metal Surfaces. Physical Review Letters, 2007, 99, 016105.	2.9	1,270
6	A theoretical evaluation of possible transition metal electro-catalysts for N₂reduction. Physical Chemistry Chemical Physics, 2012, 14, 1235-1245.	1.3	1,184
7	Identification of Non-Precious Metal Alloy Catalysts for Selective Hydrogenation of Acetylene. Science, 2008, 320, 1320-1322.	6.0	984
8	Discovery of a Ni-Ga catalyst for carbon dioxide reduction to methanol. Nature Chemistry, 2014, 6, 320-324.	6.6	865
9	Structure effects on the energetics of the electrochemical reduction of CO2 by copper surfaces. Surface Science, 2011, 605, 1354-1359.	0.8	445
10	The Mechanism of CO and CO₂ Hydrogenation to Methanol over Cuâ€Based Catalysts. ChemCatChem, 2015, 7, 1105-1111.	1.8	424
11	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
12	Understanding trends in Câ€“H bond activation in heterogeneous catalysis. Nature Materials, 2017, 16, 225-229.	13.3	387
13	Exploring the limits: A low-pressure, low-temperature Haberâ€“Bosch process. Chemical Physics Letters, 2014, 598, 108-112.	1.2	369
14	Universal transition state scaling relations for (de)hydrogenation over transition metals. Physical Chemistry Chemical Physics, 2011, 13, 20760.	1.3	363
15	Theory-guided design of catalytic materials using scaling relationships and reactivity descriptors. Nature Reviews Materials, 2019, 4, 792-804.	23.3	338
16	Understanding activity trends in electrochemical water oxidation to form hydrogen peroxide. Nature Communications, 2017, 8, 701.	5.8	333
17	Assessing the reliability of calculated catalytic ammonia synthesis rates. Science, 2014, 345, 197-200.	6.0	319
18	Electrochemical chlorine evolution at rutile oxide (110) surfaces. Physical Chemistry Chemical Physics, 2010, 12, 283-290.	1.3	317

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19	Theoretical Insight into the Trends that Guide the Electrochemical Reduction of Carbon Dioxide to Formic Acid. ChemSusChem, 2016, 9, 358-363.	3.6	311
20	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
21	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
22	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
23	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
24	Theoretical Analysis of Transition-Metal Catalysts for Formic Acid Decomposition. ACS Catalysis, 2014, 4, 1226-1233.	5.5	209
25	Tracking the formation, fate and consequence for catalytic activity of Pt single sites on CeO2. Nature Catalysis, 2020, 3, 824-833.	16.1	209
26	CO hydrogenation to methanol on Cuâ€“Ni catalysts: Theory and experiment. Journal of Catalysis, 2012, 293, 51-60.	3.1	195
27	Intrinsic Selectivity and Structure Sensitivity of Rhodium Catalysts for C₂₊ Oxygenate Production. Journal of the American Chemical Society, 2016, 138, 3705-3714.	6.6	179
28	Activity and Selectivity Trends in Synthesis Gas Conversion to Higher Alcohols. Topics in Catalysis, 2014, 57, 135-142.	1.3	173
29	Monocopper Active Site for Partial Methane Oxidation in Cu-Exchanged 8MR Zeolites. ACS Catalysis, 2016, 6, 6531-6536.	5.5	173
30	Energetics and Mechanism of a Room-Temperature Catalytic Process for Ammonia Synthesis (Schrock) Tj ETQq0 0 0 rgBT /Overlock 10 T 2005, 44, 5639-5642.	7.2	151
31	CO and CO2 Hydrogenation to Methanol Calculated Using the BEEF-vdW Functional. Catalysis Letters, 2013, 143, 71-73.	1.4	148
32	Theoretical Insights into the Selective Oxidation of Methane to Methanol in Copper-Exchanged Mordenite. ACS Catalysis, 2016, 6, 3760-3766.	5.5	139
33	Cation-exchanged zeolites for the selective oxidation of methane to methanol. Catalysis Science and Technology, 2018, 8, 114-123.	2.1	135
34	On the behavior of BrÃ¸nsted-Evans-Polanyi relations for transition metal oxides. Journal of Chemical Physics, 2011, 134, 244509.	1.2	128
35	CatApp: A Web Application for Surface Chemistry and Heterogeneous Catalysis. Angewandte Chemie - International Edition, 2012, 51, 272-274.	7.2	126
36	Theoretical, spectroscopic, and mechanistic studies on transition-metal dinitrogen complexes: Implications to reactivity and relevance to the nitrogenase problem. Journal of Computational Chemistry, 2006, 27, 1278-1291.	1.5	119

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37	Unraveling the Mechanism of the Initiation Reaction of the Methanol to Olefins Process Using ab Initio and DFT Calculations. ACS Catalysis, 2017, 7, 7987-7994.	5.5	118
38	Unlocking synergy in bimetallic catalysts by coreâ€“shell design. Nature Materials, 2021, 20, 1216-1220.	13.3	111
39	Scaling relationships for adsorption energies of C2 hydrocarbons on transition metal surfaces. Chemical Engineering Science, 2011, 66, 6318-6323.	1.9	108
40	Degree of rate control approach to computational catalyst screening. Journal of Catalysis, 2015, 330, 197-207.	3.1	105
41	Ketene as a Reaction Intermediate in the Carbonylation of Dimethyl Ether to Methyl Acetate over Mordenite. Angewandte Chemie - International Edition, 2015, 54, 7261-7264.	7.2	98
42	Prospects of Heterogeneous Hydroformylation with Supported Single Atom Catalysts. Journal of the American Chemical Society, 2020, 142, 5087-5096.	6.6	98
43	Elementary steps of syngas reactions on Mo2C(001): Adsorption thermochemistry and bond dissociation. Journal of Catalysis, 2012, 290, 108-117.	3.1	96
44	Reactivity Descriptor in Solid Acid Catalysis: Predicting Turnover Frequencies for Propene Methylation in Zeotypes. Journal of Physical Chemistry Letters, 2014, 5, 1516-1521.	2.1	96
45	Effect of Boron Modifications of Palladium Catalysts for the Production of Hydrogen from Formic Acid. ACS Catalysis, 2015, 5, 6579-6586.	5.5	88
46	Mechanistic insights into nitrogen fixation by nitrogenase enzymes. Physical Chemistry Chemical Physics, 2015, 17, 29541-29547.	1.3	84
47	Descriptorâ€Based Analysis Applied to HCN Synthesis from NH₃ and CH₄. Angewandte Chemie - International Edition, 2011, 50, 4601-4605.	7.2	80
48	DFT-Based Method for More Accurate Adsorption Energies: An Adaptive Sum of Energies from RPBE and vdW Density Functionals. Journal of Physical Chemistry C, 2017, 121, 4937-4945.	1.5	80
49	Energetics and Mechanism of Ammonia Synthesis through the Chatt Cycle: Conditions for a Catalytic Mode and Comparison with the Schrock Cycle. Chemistry - A European Journal, 2008, 14, 644-652.	1.7	77
50	Photothermal Catalysis over Nonplasmonic Pt/TiO₂ Studied by Operando HERFD-XANES, Resonant XES, and DRIFTS. ACS Catalysis, 2018, 8, 11398-11406.	5.5	76
51	Oneâ€Pot Cooperation of Singleâ€Atom Rh and Ru Solid Catalysts for a Selective Tandem Olefin Isomerizationâ€Hydrosilylation Process. Angewandte Chemie - International Edition, 2020, 59, 5806-5815.	7.2	76
52	Metal-Specific Reactivity in Single-Atom Catalysts: CO Oxidation on 4d and 5d Transition Metals Atomically Dispersed on MgO. Journal of the American Chemical Society, 2020, 142, 14890-14902.	6.6	75
53	Methanolâ€“Alkene Reactions in Zeotype Acid Catalysts: Insights from a Descriptor-Based Approach and Microkinetic Modeling. ACS Catalysis, 2014, 4, 4504-4509.	5.5	74
54	Interplay of Electronic and Steric Effects to Yield Lowâ€Temperature CO Oxidation at Metal Single Sites in Defectâ€Engineered HKUSTâ€1. Angewandte Chemie - International Edition, 2020, 59, 10514-10518.	7.2	73

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55	The Oxygen Reduction Reaction on Nitrogen-Doped Graphene. Catalysis Letters, 2013, 143, 58-60.	1.4	69
56	A Highly Active Molybdenum Phosphide Catalyst for Methanol Synthesis from CO and CO₂. Angewandte Chemie - International Edition, 2018, 57, 15045-15050.	7.2	69
57	High-performance oxygen reduction and evolution carbon catalysis: From mechanistic studies to device integration. Nano Research, 2017, 10, 1163-1177.	5.8	66
58	Selectivity of Synthesis Gas Conversion to C₂₊ Oxygenates on fcc(111) Transition-Metal Surfaces. ACS Catalysis, 2018, 8, 3447-3453.	5.5	66
59	In silicosearch for novel methane steam reforming catalysts. New Journal of Physics, 2013, 15, 125021.	1.2	65
60	A systematic study of metal-supported boron nitride materials for the oxygen reduction reaction. Physical Chemistry Chemical Physics, 2015, 17, 12722-12727.	1.3	65
61	Combined In Situ EDXRD/EXAFS Investigation of the Crystal Growth of [Co(C6H18N4)][Sb2S4] under Solvothermal Conditions:Â Two Different Reaction Pathways Leading to the Same Product. Chemistry of Materials, 2006, 18, 1196-1205.	3.2	64
62	Identification of the Reaction Sequence of the MTO Initiation Mechanism Using Ab Initio-Based Kinetics. Journal of the American Chemical Society, 2019, 141, 5908-5915.	6.6	64
63	Energetics of Oxygen Adatoms, Hydroxyl Species and Water Dissociation on Pt(111). Journal of Physical Chemistry C, 2012, 116, 25772-25776.	1.5	62
64	Hydrodeoxygenation of Phenol to Benzene and Cyclohexane on Rh(111) and Rh(211) Surfaces: Insights from Density Functional Theory. Journal of Physical Chemistry C, 2016, 120, 18529-18537.	1.5	61
65	Two-Dimensional Materials as Catalysts for Energy Conversion. Catalysis Letters, 2016, 146, 1917-1921.	1.4	58
66	Transition-state scaling relations in zeolite catalysis: influence of framework topology and acid-site reactivity. Catalysis Science and Technology, 2015, 5, 2814-2820.	2.1	56
67	On the Accuracy of Density Functional Theory in Zeolite Catalysis. ChemCatChem, 2019, 11, 4368-4376.	1.8	55
68	Thermochemistry and micro-kinetic analysis of methanol synthesis on ZnO (0 0 0 1). Journal of Catalysis, 2014, 309, 397-407.	3.1	54
69	Reaction mechanism of dimethyl ether carbonylation to methyl acetate over mordenite â€“ a combined DFT/experimental study. Catalysis Science and Technology, 2017, 7, 1141-1152.	2.1	54
70	Reduction Pathway of End-On Terminally Coordinated Dinitrogen. V. Nâˆ’N Bond Cleavage in Mo/W Hydrazidium Complexes with Diphosphine Coligands. Comparison with Triamidoamine Systems. Inorganic Chemistry, 2005, 44, 3031-3045.	1.9	53
71	[Ni(C4H13N3)2]3(Sb3S6)2: The First Structure Containing Isolated Heterocyclic [Sb3S6]3âˆ’ Anions. European Journal of Inorganic Chemistry, 2004, 2004, 2553-2556.	1.0	52
72	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

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73	Exploiting Synergies in Catalysis and Gas Sensing using Noble Metalâ€Loaded Oxide Composites. ChemCatChem, 2018, 10, 864-880.	1.8	50
74	Volcano Relation for the Deacon Process over Transitionâ€Metal Oxides. ChemCatChem, 2010, 2, 98-102.	1.8	49
75	Structural dynamics in Niâ€“Fe catalysts during CO₂ methanation â€“ role of iron oxide clusters. Catalysis Science and Technology, 2020, 10, 7542-7554.	2.1	48
76	Spectroscopic Properties and Quantum Chemistry-Based Normal Coordinate Analysis (QCB-NCA) of a Dinuclear Tantalum Complex Exhibiting the Novel Side-On End-On Bridging Geometry of N2:Â Correlations to Electronic Structure and Reactivity. Journal of the American Chemical Society, 2004, 126, 280-290.	6.6	47
77	Theoretical Insights into the Effect of the Framework on the Initiation Mechanism of the MTO Process. Catalysis Letters, 2018, 148, 1246-1253.	1.4	46
78	Metal Oxideâ€Supported Platinum Overlayers as Protonâ€Exchange Membrane Fuel Cell Cathodes. ChemCatChem, 2012, 4, 228-235.	1.8	44
79	Probing the Active Sites of MoS₂ Based Hydrotreating Catalysts Using Modulation Excitation Spectroscopy. ACS Catalysis, 2019, 9, 2568-2579.	5.5	43
80	Lewis Adducts of the Side-On End-On Dinitrogen-Bridged Complex [{(NPN)Ta}2(?-H)2(?-?1:?2-N2)] with AlMe3, GaMe3, and B(C6F5)3: Synthesis, Structure, and Spectroscopic Properties. Chemistry - A European Journal, 2005, 11, 604-618.	1.7	42
81	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
82	Impact of Ni promotion on the hydrogenation pathways of phenanthrene on MoS2/Î³-Al2O3. Journal of Catalysis, 2017, 352, 171-181.	3.1	38
83	Theoretical Investigation of the Acid Catalyzed Formation of Oxymethylene Dimethyl Ethers from Trioxane and Dimethoxymethane. ACS Catalysis, 2017, 7, 3615-3621.	5.5	37
84	Rendering Photoreactivity to Ceria: The Role of Defects. Angewandte Chemie - International Edition, 2017, 56, 14301-14305.	7.2	37
85	Moving Frontiers in Transition Metal Catalysis: Synthesis, Characterization and Modeling. Advanced Materials, 2019, 31, e1807381.	11.1	36
86	Theoretical Investigation of Methane Oxidation on Pd(111) and Other Metallic Surfaces. Journal of Physical Chemistry C, 2018, 122, 16023-16032.	1.5	34
87	Influence of H 2 O and H 2 S on the composition, activity, and stability of sulfided Mo, CoMo, and NiMo supported on MgAl 2 O 4 for hydrodeoxygenation of ethylene glycol. Applied Catalysis A: General, 2018, 551, 106-121.	2.2	31
88	Side-On Bridging Coordination of N2: Spectroscopic Characterization of the Planar Zr2N2 Core and Theoretical Investigation of Its Butterfly Distortion. Chemistry - A European Journal, 2003, 9, 520-530.	1.7	29
89	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
90	The Stability of Copper Oxo Species in Zeolite Frameworks. European Journal of Inorganic Chemistry, 2016, 2016, 1514-1520.	1.0	29

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91	Anharmonic Correction to Adsorption Free Energy from DFT-Based MD Using Thermodynamic Integration. Journal of Chemical Theory and Computation, 2021, 17, 1155-1169.	2.3	29
92	Adsorption Preference Determines Segregation Direction: A Shortcut to More Realistic Surface Models of Alloy Catalysts. ACS Catalysis, 2019, 9, 5011-5018.	5.5	27
93	How Accurately Do Approximate Density Functionals Predict Trends in Acidic Zeolite Catalysis?. Journal of Physical Chemistry Letters, 2020, 11, 4305-4310.	2.1	27
94	Shape-Selective Synthesis of Intermetallic Pd₃Pb Nanocrystals and Enhanced Catalytic Properties in the Direct Synthesis of Hydrogen Peroxide. ACS Catalysis, 2021, 11, 2288-2301.	5.5	27
95	Different routes to methanol: inelastic neutron scattering spectroscopy of adsorbates on supported copper catalysts. Physical Chemistry Chemical Physics, 2016, 18, 17253-17258.	1.3	26
96	Olefin methylation and cracking reactions in H-SSZ-13 investigated with ab initio and DFT calculations. Catalysis Science and Technology, 2018, 8, 4420-4429.	2.1	26
97	Computer-Generated Kinetics for Coupled Heterogeneous/Homogeneous Systems: A Case Study in Catalytic Combustion of Methane on Platinum. Industrial & Engineering Chemistry Research, 2019, 58, 17682-17691.	1.8	26
98	Using microkinetic analysis to search for novel anhydrous formaldehyde production catalysts. Surface Science, 2015, 641, 105-111.	0.8	25
99	Scaling Relationships for Binding Energies of Transition Metal Complexes. Catalysis Letters, 2016, 146, 304-308.	1.4	25
100	On the Reactivity of the Cu/ZrO₂ System for the Hydrogenation of CO₂ to Methanol: A Density Functional Theory Study. Journal of Physical Chemistry C, 2019, 123, 26904-26911.	1.5	24
101	Thermal Defect Engineering of Precious Group Metalâ€“Organic Frameworks: A Case Study on Ru/Rh-HKUST-1 Analogues. ACS Applied Materials & Interfaces, 2020, 12, 40635-40647.	4.0	24
102	Supported Intermetallic PdZn Nanoparticles as Bifunctional Catalysts for the Direct Synthesis of Dimethyl Ether from COâ€Rich Synthesis Gas. Angewandte Chemie - International Edition, 2019, 58, 15655-15659.	7.2	23
103	Spectroscopic Comparison of Dinuclear Ti+ and Ti2+ Î¼-Î·1:Î·1 Dinitrogen Complexes with Cp*/Pentafulvene and Amine/Amide Ligation: Moderate versus Strong Activation of N2. European Journal of Inorganic Chemistry, 2006, 2006, 291-297.	1.0	22
104	Enhanced Direct Dimethyl Ether Synthesis from CO2-Rich Syngas with Cu/ZnO/ZrO2 Catalysts Prepared by Continuous Co-Precipitation. Catalysts, 2020, 10, 816.	1.6	22
105	A Systematic Study of Methylation from Benzene to Hexamethylbenzene in H-SSZ-13 Using Density Functional Theory and Ab Initio Calculations. ACS Catalysis, 2020, 10, 8916-8925.	5.5	21
106	Influence of Acidity on the Methanol-to-DME Reaction in Zeotypes: A First Principles-Based Microkinetic Study. Journal of Physical Chemistry C, 2020, 124, 14658-14663.	1.5	21
107	Oneâ€Pot Cooperation of Singleâ€Atom Rh and Ru Solid Catalysts for a Selective Tandem Olefin Isomerizationâ€Hydrosilylation Process. Angewandte Chemie, 2020, 132, 5855-5864.	1.6	21
108	Grand Challenges in Computational Catalysis. Frontiers in Catalysis, 2021, 1, .	1.8	21

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109	Application of a Universal Force Field to Mixed Fe/Moâ˜S/Se Cubane and Heterocubane Clusters. 1. Substitution of Sulfur by Selenium in the Series [Fe4X4(YCH3)4]2-; X = S/Se and Y = S/Seâ€. Inorganic Chemistry, 2004, 43, 5003-5010.	1.9	20
110	Modeling the Size Dependency of the Stability of Metal Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 25464-25469.	1.5	20
111	NH₃-SCR over Vâ€“W/TiO₂ Investigated by Operando X-ray Absorption and Emission Spectroscopy. Journal of Physical Chemistry C, 2019, 123, 14338-14349.	1.5	20
112	Unravelling the Znâ€Cu Interaction during Activation of a Znâ€promoted Cu/MgO Model Methanol Catalyst. ChemCatChem, 2021, 13, 4120-4132.	1.8	20
113	Surface reaction kinetics of the methanol synthesis and the water gas shift reaction on Cu/ZnO/Al₂O₃. Reaction Chemistry and Engineering, 2021, 6, 868-887.	1.9	20
114	Surface Noble Metal Concentration on Ceria as a Key Descriptor for Efficient Catalytic CO Oxidation. ACS Catalysis, 2022, 12, 2473-2486.	5.5	19
115	Nâ€“N splitting of a functionalized Âµ-Î·1:Î·2coordinated N2ligand leading to a Âµ-nitrido Âµ-imido core: mechanistic insight from DFT. Dalton Transactions, 2006, , 1137-1140.	1.6	18
116	Exploring Scaling Relations for Chemisorption Energies on Transitionâ€Metalâ€Exchanged Zeolites ZSMâ€22 and ZSMâ€5. ChemCatChem, 2016, 8, 767-772.	1.8	18
117	Dynamic structural changes of supported Pd, PdSn, and PdIn nanoparticles during continuous flow high pressure direct H₂O₂ synthesis. Catalysis Science and Technology, 2020, 10, 4726-4742.	2.1	17
118	Mechanistic differences between methanol and dimethyl ether in zeolite-catalyzed hydrocarbon synthesis. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	17
119	Vibrational and electronic structure of the dinuclear bis(Âµ-nitrido) vanadium(v) complex [V(N{Nâ€³}2)(Âµ-N)]2: spectroscopic properties of the M2(Âµ-N)2diamond core. Dalton Transactions, 2005, , 1052-1057.	1.6	16
120	Bottomâ€Up Design of a Copperâ€Ruthenium Nanoparticulate Catalyst for Lowâ€Temperature Ammonia Oxidation. Angewandte Chemie - International Edition, 2017, 56, 8711-8715.	7.2	16
121	Moderate Surface Segregation Promotes Selective Ethanol Production in CO₂Hydrogenation Reaction over CoCu Catalysts. Angewandte Chemie - International Edition, 2022, 61, .	7.2	16
122	Reactivity of Surface Lewis and BrÃ¸nsted Acid Sites in Zeolite Catalysis: A Computational Case Study of DME Synthesis Using H-SSZ-13. Journal of Physical Chemistry C, 2022, 126, 5896-5905.	1.5	16
123	Trends in the Hydrodeoxygenation Activity and Selectivity of Transition Metal Surfaces. Catalysis Letters, 2014, 144, 1968-1972.	1.4	15
124	A Highly Active Molybdenum Phosphide Catalyst for Methanol Synthesis from CO and CO₂. Angewandte Chemie, 2018, 130, 15265-15270.	1.6	15
125	Simple Scheme to Predict Transition-State Energies of Dehydration Reactions in Zeolites with Relevance to Biomass Conversion. Journal of Physical Chemistry C, 2018, 122, 23062-23067.	1.5	14
126	Orbital Interactions in Fe(II)/Co(III) Heterobimetallocenes:Â Single versus Double Bridge. Inorganic Chemistry, 2006, 45, 2531-2542.	1.9	13

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127	High Pressure CO Hydrogenation Over Bimetallic Ptâ€“Co Catalysts. Catalysis Letters, 2014, 144, 777-782.	1.4	13
128	Predicting Promoter-Induced Bond Activation on Solid Catalysts Using Elementary Bond Orders. Journal of Physical Chemistry Letters, 2015, 6, 3670-3674.	2.1	13
129	Catalysis by unusual vacancies. Nature Catalysis, 2021, 4, 184-185.	16.1	13
130	Methanol Partial Oxidation on Ag(1â€‰1â€‰1) from First Principles. ChemCatChem, 2016, 8, 3621-3625.	1.8	12
131	Theoretical investigation of the side-chain mechanism of the MTO process over H-SSZ-13 using DFT and ab initio calculations. Catalysis Science and Technology, 2021, 11, 3826-3833.	2.1	12
132	Dismutation of a Molybdenum(IV) Acetonitrileâ¯NNH2Complex to a Molybdenum(IV) Ethylimido Complex + N2:Â Mechanistic Implications on the Protonation of Coordinated Nitriles at the Î²-Carbon Atom. Organometallics, 2005, 24, 5393-5406.	1.1	11
133	Volcano Relations for Oxidation of Hydrogen Halides over Rutile Oxide Surfaces. ChemCatChem, 2012, 4, 1856-1861.	1.8	11
134	Trends in Adsorption Energies of the Oxygenated Species on Single Platinum Atom Embedded in Carbon Nanotubes. Catalysis Letters, 2017, 147, 2689-2696.	1.4	10
135	Trends in the Activation of Light Alkanes on Transition-Metal Surfaces. Journal of Physical Chemistry C, 2020, 124, 27503-27510.	1.5	10
136	Theoretical Study on the NO_x Selective Catalytic Reduction on Single-Cu Sites and BrÃ¸nsted Acid Sites in Cu-SSZ-13. Journal of Physical Chemistry C, 2021, 125, 12594-12602.	1.5	10
137	Bottomâ€Up Design of a Copperâ€“Ruthenium Nanoparticulate Catalyst for Lowâ€Temperature Ammonia Oxidation. Angewandte Chemie, 2017, 129, 8837-8841.	1.6	9
138	Zusammenwirken elektronischer und sterischer Effekte bei der Tieftemperaturâ€COâ€Oxidation an Einzelatomâ€Metallzentren in defektâ€manipuliertem HKUSTâ€1. Angewandte Chemie, 2020, 132, 10600-10604.	1.6	9
139	Density functional theory calculations of diffusion barriers of organic molecules through the 8-ring of H-SSZ-13. Chemical Physics, 2021, 541, 111033.	0.9	9
140	Discovering the role of substrate in aldehyde hydrogenation. Journal of Catalysis, 2021, 399, 162-169.	3.1	9
141	Theoretical Investigations of (Oxidative) Dehydrogenation of Propane to Propylene over Palladium Surfaces. Journal of Physical Chemistry C, 2020, 124, 3171-3176.	1.5	8
142	Analysis of sulfur-induced selectivity changes for anhydrous methanol dehydrogenation on Ni(100) surfaces. Surface Science, 2013, 613, 58-62.	0.8	7
143	Supported Intermetallic PdZn Nanoparticles as Bifunctional Catalysts for the Direct Synthesis of Dimethyl Ether from COâ€Rich Synthesis Gas. Angewandte Chemie, 2019, 131, 15802-15806.	1.6	7
144	Trends in the Reactivity of Proximate Aluminum Sites in H-SSZ-13. Journal of Physical Chemistry C, 2021, 125, 16508-16515.	1.5	7

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145	A new mechanistic proposal for the aromatic cycle of the MTO process based on a computational investigation for H-SSZ-13. Catalysis Science and Technology, 2022, 12, 3516-3523.	2.1	7
146	Can Single Metal Atoms Trapped in Defective h-BN/Cu(111) Improve Electrocatalysis of the H₂ Evolution Reaction?. Journal of Physical Chemistry C, 2020, 124, 23690-23698.	1.5	6
147	Influence of Confinement on Barriers for Alkoxide Formation in Acidic Zeolites. ChemCatChem, 2021, 13, 2451-2458.	1.8	6
148	Effect of Aluminum Siting in H-ZSM-5 on Reaction Barriers. Journal of Physical Chemistry C, 2021, 125, 20373-20379.	1.5	6
149	A Computational Investigation of OMEâ€synthesis through Homogeneous Acid Catalysis. ChemCatChem, 2019, 11, 1949-1954.	1.8	5
150	Effect of Impurities on the Initiation of the Methanol-to-Olefins Process: Kinetic Modeling Based on Ab Initio Rate Constants. Catalysis Letters, 2021, 151, 2595-2602.	1.4	4
151	Theoretical Investigation of the Size Effect on the Oxygen Adsorption Energy of Coinage Metal Nanoparticles. Catalysis Letters, 2021, 151, 3165-3169.	1.4	4
152	The barrier free splitting of O-H bond in H2O and CH3OH due to the synergetic effects of single atom (Cu1/Fe1) coordination change and ZnO(1 1 0) surface oxygen activation. Applied Surface Science, 2022, 576, 151750.	3.1	3
153	Theoretical investigation of the olefin cycle in H-SSZ-13 for the ethanol-to-olefins process using ab initio calculations and kinetic modeling. Catalysis Science and Technology, 2022, 12, 3311-3321.	2.1	2
154	N₂O Adsorption and Photochemistry on Ceria Surfaces. Journal of Physical Chemistry C, 2022, 126, 2253-2263.	1.5	1
155	[Ni(C4H13N3)2]3(Sb3S6)2: The First Structure Containing Isolated Heterocyclic [Sb3S6]3- Anions.. ChemInform, 2004, 35, no.	0.1	0
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