Felix Studt

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

161 papers	17,443 citations	54 h-index	131 g-index
175 ext. papers	20,617 ext. citations	8.8 avg, IF	6.88 L-index

#	Paper	IF	Citations
161	N2O Adsorption and Photochemistry on Ceria Surfaces. *Journal of Physical Chemistry C*, **2022**, 126, 2253-2263	3.8	0
160	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,	11.5	3
159	Reactivity of Surface Lewis and Brønsted 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	3.8	4
158	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(110) surface oxygen activation. *Applied Surface Science*, **2021**, 151750	6.7	0
157	Influence of Confinement on Barriers for Alkoxide Formation in Acidic Zeolites. *ChemCatChem*, **2021**, 13, 2451-2458	5.2	1
156	Grand Challenges in Computational Catalysis. *Frontiers in Catalysis*, **2021**, 1,		5
155	Unlocking synergy in bimetallic catalysts by core-shell design. *Nature Materials*, **2021**, 20, 1216-1220	27	30
154	Theoretical Study on the NOx Selective Catalytic Reduction on Single-Cu Sites and Brønsted Acid Sites in Cu-SSZ-13. *Journal of Physical Chemistry C*, **2021**, 125, 12594-12602	3.8	2
153	Trends in the Reactivity of Proximate Aluminum Sites in H-SSZ-13. *Journal of Physical Chemistry C*, **2021**, 125, 16508-16515	3.8	5
152	Discovering the role of substrate in aldehyde hydrogenation. *Journal of Catalysis*, **2021**, 399, 162-169	7.3	2
151	Density functional theory calculations of diffusion barriers of organic molecules through the 8-ring of H-SSZ-13. *Chemical Physics*, **2021**, 541, 111033	2.3	6
150	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	5.5	4
149	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	2.8	3
148	Theoretical Investigation of the Size Effect on the Oxygen Adsorption Energy of Coinage Metal Nanoparticles. *Catalysis Letters*, **2021**, 151, 3165-3169	2.8	1
147	Shape-Selective Synthesis of Intermetallic Pd3Pb Nanocrystals and Enhanced Catalytic Properties in the Direct Synthesis of Hydrogen Peroxide. *ACS Catalysis*, **2021**, 11, 2288-2301	13.1	12
146	Unravelling the Zn-Cu Interaction during Activation of a Zn-promoted Cu/MgO Model Methanol Catalyst. *ChemCatChem*, **2021**, 13, 4120	5.2	7
145	Effect of Aluminum Siting in H-ZSM-5 on Reaction Barriers. *Journal of Physical Chemistry C*, **2021**, 125, 20373-20379	3.8	2

144	Anharmonic Correction to Adsorption Free Energy from DFT-Based MD Using Thermodynamic Integration. *Journal of Chemical Theory and Computation*, **2021**, 17, 1155-1169	6.4	14
143	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	4.9	6
142	Zusammenwirken elektronischer und sterischer Effekte bei der Tieftemperatur-CO-Oxidation an Einzelatom-Metallzentren in defekt-manipuliertem HKUST-1. *Angewandte Chemie*, **2020**, 132, 10600-10604	3.6	5
141	How Accurately Do Approximate Density Functionals Predict Trends in Acidic Zeolite Catalysis?. *Journal of Physical Chemistry Letters*, **2020**, 11, 4305-4310	6.4	16
140	Interplay of Electronic and Steric Effects to Yield Low-Temperature CO Oxidation at Metal Single Sites in Defect-Engineered HKUST-1. *Angewandte Chemie - International Edition*, **2020**, 59, 10514-10518	16.4	34
139	Prospects of Heterogeneous Hydroformylation with Supported Single Atom Catalysts. *Journal of the American Chemical Society*, **2020**, 142, 5087-5096	16.4	45
138	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	5.5	10
137	One-Pot Cooperation of Single-Atom Rh and Ru Solid Catalysts for a Selective Tandem Olefin Isomerization-Hydrosilylation Process. *Angewandte Chemie*, **2020**, 132, 5855-5864	3.6	10
136	Theoretical Investigations of (Oxidative) Dehydrogenation of Propane to Propylene over Palladium Surfaces. *Journal of Physical Chemistry C*, **2020**, 124, 3171-3176	3.8	6
135	One-Pot Cooperation of Single-Atom Rh and Ru Solid Catalysts for a Selective Tandem Olefin Isomerization-Hydrosilylation Process. *Angewandte Chemie - International Edition*, **2020**, 59, 5806-5815	16.4	41
134	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	3.8	1
133	Structural dynamics in NiFe catalysts during CO2 methanation – role of iron oxide clusters. *Catalysis Science and Technology*, **2020**, 10, 7542-7554	5.5	19
132	Trends in the Activation of Light Alkanes on Transition-Metal Surfaces. *Journal of Physical Chemistry C*, **2020**, 124, 27503-27510	3.8	3
131	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	13.1	12
130	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	16.4	40
129	Thermal Defect Engineering of Precious Group Metal-Organic Frameworks: A Case Study on Ru/Rh-HKUST-1 Analogues. *ACS Applied Materials & Interfaces*, **2020**, 12, 40635-40647	9.5	10
128	Tracking the formation, fate and consequence for catalytic activity of Pt single sites on CeO2. *Nature Catalysis*, **2020**, 3, 824-833	36.5	84
127	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	3.8	12

126	Enhanced Direct Dimethyl Ether Synthesis from CO2-Rich Syngas with Cu/ZnO/ZrO2 Catalysts Prepared by Continuous Co-Precipitation. *Catalysts*, **2020**, 10, 816	4	5
125	Supported Intermetallic PdZn Nanoparticles as Bifunctional Catalysts for the Direct Synthesis of Dimethyl Ether from CO-Rich Synthesis Gas. *Angewandte Chemie*, **2019**, 131, 15802-15806	3.6	6
124	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	3.9	16
123	Modeling the Size Dependency of the Stability of Metal Nanoparticles. *Journal of Physical Chemistry C*, **2019**, 123, 25464-25469	3.8	15
122	Probing the Active Sites of MoS2 Based Hydrotreating Catalysts Using Modulation Excitation Spectroscopy. *ACS Catalysis*, **2019**, 9, 2568-2579	13.1	28
121	NH3-SCR over V□W/TiO2 Investigated by Operando X-ray Absorption and Emission Spectroscopy. *Journal of Physical Chemistry C*, **2019**, 123, 14338-14349	3.8	17
120	Transition Metal Catalysis: Moving Frontiers in Transition Metal Catalysis: Synthesis, Characterization and Modeling (Adv. Mater. 26/2019). *Advanced Materials*, **2019**, 31, 1970187	24	
119	Adsorption Preference Determines Segregation Direction: A Shortcut to More Realistic Surface Models of Alloy Catalysts. *ACS Catalysis*, **2019**, 9, 5011-5018	13.1	19
118	A Computational Investigation of OME-synthesis through Homogeneous Acid Catalysis. *ChemCatChem*, **2019**, 11, 1949-1954	5.2	3
117	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	16.4	30
116	Moving Frontiers in Transition Metal Catalysis: Synthesis, Characterization and Modeling. *Advanced Materials*, **2019**, 31, e1807381	24	29
115	Supported Intermetallic PdZn Nanoparticles as Bifunctional Catalysts for the Direct Synthesis of Dimethyl Ether from CO-Rich Synthesis Gas. *Angewandte Chemie - International Edition*, **2019**, 58, 15655-15659	16.4	18
114	On the Accuracy of Density Functional Theory in Zeolite Catalysis. *ChemCatChem*, **2019**, 11, 4368-4376	5.2	34
113	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	3.8	13
112	Theory-guided design of catalytic materials using scaling relationships and reactivity descriptors. *Nature Reviews Materials*, **2019**, 4, 792-804	73.3	164
111	Theoretical Insights into the Effect of the Framework on the Initiation Mechanism of the MTO Process. *Catalysis Letters*, **2018**, 148, 1246-1253	2.8	35
110	Selectivity of Synthesis Gas Conversion to C2+ Oxygenates on fcc(111) Transition-Metal Surfaces. *ACS Catalysis*, **2018**, 8, 3447-3453	13.1	48
109	Cation-exchanged zeolites for the selective oxidation of methane to methanol. *Catalysis Science and Technology*, **2018**, 8, 114-123	5.5	110

108	Theoretical Investigation of Methane Oxidation on Pd(111) and Other Metallic Surfaces. *Journal of Physical Chemistry C*, **2018**, 122, 16023-16032	3.8	21
107	A Highly Active Molybdenum Phosphide Catalyst for Methanol Synthesis from CO and CO2. *Angewandte Chemie*, **2018**, 130, 15265-15270	3.6	12
106	Olefin methylation and cracking reactions in H-SSZ-13 investigated with ab initio and DFT calculations. *Catalysis Science and Technology*, **2018**, 8, 4420-4429	5.5	18
105	A Highly Active Molybdenum Phosphide Catalyst for Methanol Synthesis from CO and CO. *Angewandte Chemie - International Edition*, **2018**, 57, 15045-15050	16.4	46
104	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	5.1	21
103	Exploiting Synergies in Catalysis and Gas Sensing using Noble Metal-Loaded Oxide Composites. *ChemCatChem*, **2018**, 10, 864-880	5.2	39
102	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	3.8	8
101	Photothermal Catalysis over Nonplasmonic Pt/TiO2 Studied by Operando HERFD-XANES, Resonant XES, and DRIFTS. *ACS Catalysis*, **2018**, 8, 11398-11406	13.1	49
100	Reaction mechanism of dimethyl ether carbonylation to methyl acetate over mordenite combined DFT/experimental study. *Catalysis Science and Technology*, **2017**, 7, 1141-1152	5.5	35
99	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	3.8	54
98	Theoretical Investigation of the Acid Catalyzed Formation of Oxymethylene Dimethyl Ethers from Trioxane and Dimethoxymethane. *ACS Catalysis*, **2017**, 7, 3615-3621	13.1	27
97	Bottom-Up Design of a Copper-Ruthenium Nanoparticulate Catalyst for Low-Temperature Ammonia Oxidation. *Angewandte Chemie - International Edition*, **2017**, 56, 8711-8715	16.4	12
96	High-performance oxygen reduction and evolution carbon catalysis: From mechanistic studies to device integration. *Nano Research*, **2017**, 10, 1163-1177	10	50
95	Impact of Ni promotion on the hydrogenation pathways of phenanthrene on MoS2/Al2O3. *Journal of Catalysis*, **2017**, 352, 171-181	7.3	30
94	Bottom-Up Design of a CopperRuthenium Nanoparticulate Catalyst for Low-Temperature Ammonia Oxidation. *Angewandte Chemie*, **2017**, 129, 8837-8841	3.6	7
93	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	13.1	80
92	Trends in Adsorption Energies of the Oxygenated Species on Single Platinum Atom Embedded in Carbon Nanotubes. *Catalysis Letters*, **2017**, 147, 2689-2696	2.8	10
91	Understanding activity trends in electrochemical water oxidation to form hydrogen peroxide. *Nature Communications*, **2017**, 8, 701	17.4	193

90	Rendering Photoreactivity to Ceria: The Role of Defects. *Angewandte Chemie - International Edition*, **2017**, 56, 14301-14305	16.4	28
89	Understanding trends in C-H bond activation in heterogeneous catalysis. *Nature Materials*, **2017**, 16, 225-229	27	276
88	Two-Dimensional Materials as Catalysts for Energy Conversion. *Catalysis Letters*, **2016**, 146, 1917-1921	2.8	39
87	Monocopper Active Site for Partial Methane Oxidation in Cu-Exchanged 8MR Zeolites. *ACS Catalysis* , **2016**, 6, 6531-6536	13.1	136
86	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	3.8	51
85	Methanol Partial Oxidation on Ag(1 1 1) from First Principles. *ChemCatChem*, **2016**, 8, 3621-3625	5.2	10
84	Exploring Scaling Relations for Chemisorption Energies on Transition-Metal-Exchanged Zeolites ZSM-22 and ZSM-5. *ChemCatChem*, **2016**, 8, 767-772	5.2	16
83	The Stability of Copper Oxo Species in Zeolite Frameworks. *European Journal of Inorganic Chemistry* , **2016**, 2016, 1514-1520	2.3	25
82	Intrinsic Selectivity and Structure Sensitivity of Rhodium Catalysts for C(2+) Oxygenate Production. *Journal of the American Chemical Society*, **2016**, 138, 3705-14	16.4	137
81	Scaling Relationships for Binding Energies of Transition Metal Complexes. *Catalysis Letters*, **2016**, 146, 304-308	2.8	18
80	Theoretical Insight into the Trends that Guide the Electrochemical Reduction of Carbon Dioxide to Formic Acid. *ChemSusChem*, **2016**, 9, 358-63	8.3	225
79	Different routes to methanol: inelastic neutron scattering spectroscopy of adsorbates on supported copper catalysts. *Physical Chemistry Chemical Physics*, **2016**, 18, 17253-8	3.6	20
78	Theoretical Insights into the Selective Oxidation of Methane to Methanol in Copper-Exchanged Mordenite. *ACS Catalysis*, **2016**, 6, 3760-3766	13.1	110
77	The Mechanism of CO and CO2 Hydrogenation to Methanol over Cu-Based Catalysts. *ChemCatChem* , **2015**, 7, 1105-1111	5.2	336
76	Using microkinetic analysis to search for novel anhydrous formaldehyde production catalysts. *Surface Science*, **2015**, 641, 105-111	1.8	22
75	Degree of rate control approach to computational catalyst screening. *Journal of Catalysis*, **2015**, 330, 197-207	7.3	82
74	A systematic study of metal-supported boron nitride materials for the oxygen reduction reaction. *Physical Chemistry Chemical Physics*, **2015**, 17, 12722-7	3.6	58
73	Ketene as a Reaction Intermediate in the Carbonylation of Dimethyl Ether to Methyl Acetate over Mordenite. *Angewandte Chemie - International Edition*, **2015**, 54, 7261-4	16.4	64

72	A benchmark database for adsorption bond energies to transition metal surfaces and comparison to selected DFT functionals. *Surface Science*, **2015**, 640, 36-44	1.8	288
71	Effect of Boron Modifications of Palladium Catalysts for the Production of Hydrogen from Formic Acid. *ACS Catalysis*, **2015**, 5, 6579-6586	13.1	68
70	Predicting Promoter-Induced Bond Activation on Solid Catalysts Using Elementary Bond Orders. *Journal of Physical Chemistry Letters*, **2015**, 6, 3670-4	6.4	12
69	Mechanistic insights into nitrogen fixation by nitrogenase enzymes. *Physical Chemistry Chemical Physics*, **2015**, 17, 29541-7	3.6	62
68	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	7.3	186
67	From the Sabatier principle to a predictive theory of transition-metal heterogeneous catalysis. *Journal of Catalysis*, **2015**, 328, 36-42	7.3	715
66	Transition-state scaling relations in zeolite catalysis: influence of framework topology and acid-site reactivity. *Catalysis Science and Technology*, **2015**, 5, 2814-2820	5.5	44
65	On the role of the surface oxygen species during A-H (A = C, N, O) bond activation: a density functional theory study. *Chemical Communications*, **2015**, 51, 2621-4	5.8	38
64	Discovery of a Ni-Ga catalyst for carbon dioxide reduction to methanol. *Nature Chemistry*, **2014**, 6, 320-4	17.6	689
63	High Pressure CO Hydrogenation Over Bimetallic Pt□o Catalysts. *Catalysis Letters*, **2014**, 144, 777-782	2.8	11
62	Activity and Selectivity Trends in Synthesis Gas Conversion to Higher Alcohols. *Topics in Catalysis*, **2014**, 57, 135-142	2.3	144
61	Thermochemistry and micro-kinetic analysis of methanol synthesis on ZnO (0 0 0 1). *Journal of Catalysis*, **2014**, 309, 397-407	7.3	46
60	Trends in the Hydrodeoxygenation Activity and Selectivity of Transition Metal Surfaces. *Catalysis Letters*, **2014**, 144, 1968-1972	2.8	12
59	Catalysis. Assessing the reliability of calculated catalytic ammonia synthesis rates. *Science*, **2014**, 345, 197-200	33.3	244
58	Theoretical Analysis of Transition-Metal Catalysts for Formic Acid Decomposition. *ACS Catalysis*, **2014**, 4, 1226-1233	13.1	169
57	Reactivity Descriptor in Solid Acid Catalysis: Predicting Turnover Frequencies for Propene Methylation in Zeotypes. *Journal of Physical Chemistry Letters*, **2014**, 5, 1516-21	6.4	85
56	**2014**,		219
55	Catalyst Structure **2014**, 138-149		

54	Poisoning and Promotion of Catalysts **2014**, 150-154		
53	Energy Trends in Catalysis **2014**, 85-96		1
52	Activity and Selectivity Maps **2014**, 97-113		0
51	Methanol–Alkene Reactions in Zeotype Acid Catalysts: Insights from a Descriptor-Based Approach and Microkinetic Modeling. *ACS Catalysis*, **2014**, 4, 4504-4509	13.1	60
50	The Potential Energy Diagram **2014**, 6-25		
49	Energetics of the Water–Gas-Shift Reaction on the Active Sites of the Industrially Used Cu/ZnO/Al2O3 Catalyst. *Catalysis Letters*, **2014**, 144, 1973-1977	2.8	23
48	Exploring the limits: A low-pressure, low-temperature Haber–Bosch process. *Chemical Physics Letters*, **2014**, 598, 108-112	2.5	275
47	Analysis of sulfur-induced selectivity changes for anhydrous methanol dehydrogenation on Ni(100) surfaces. *Surface Science*, **2013**, 613, 58-62	1.8	4
46	On the effect of coverage-dependent adsorbate–adsorbate interactions for CO methanation on transition metal surfaces. *Journal of Catalysis*, **2013**, 307, 275-282	7.3	160
45	The Oxygen Reduction Reaction on Nitrogen-Doped Graphene. *Catalysis Letters*, **2013**, 143, 58-60	2.8	65
44	CO and CO2 Hydrogenation to Methanol Calculated Using the BEEF-vdW Functional. *Catalysis Letters*, **2013**, 143, 71-73	2.8	122
43	In silicosearch for novel methane steam reforming catalysts. *New Journal of Physics*, **2013**, 15, 125021	2.9	55
42	Elementary steps of syngas reactions on Mo2C(001): Adsorption thermochemistry and bond dissociation. *Journal of Catalysis*, **2012**, 290, 108-117	7.3	84
41	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	7.3	39
40	CatApp: A Web Application for Surface Chemistry and Heterogeneous Catalysis. *Angewandte Chemie*, **2012**, 124, 278-280	3.6	26
39	CatApp: a web application for surface chemistry and heterogeneous catalysis. *Angewandte Chemie - International Edition*, **2012**, 51, 272-4	16.4	106
38	Energetics of Oxygen Adatoms, Hydroxyl Species and Water Dissociation on Pt(111). *Journal of Physical Chemistry C*, **2012**, 116, 25772-25776	3.8	54
37	CO hydrogenation to methanol on Cu–Ni catalysts: Theory and experiment. *Journal of Catalysis*, **2012**, 293, 51-60	7.3	163

36	A theoretical evaluation of possible transition metal electro-catalysts for N2 reduction. *Physical Chemistry Chemical Physics*, **2012**, 14, 1235-45	3.6	810
35	The active site of methanol synthesis over Cu/ZnO/Al2O3 industrial catalysts. *Science*, **2012**, 336, 893-7	33.3	1650
34	Metal Oxide-Supported Platinum Overlayers as Proton-Exchange Membrane Fuel Cell Cathodes. *ChemCatChem*, **2012**, 4, 228-235	5.2	42
33	Volcano Relations for Oxidation of Hydrogen Halides over Rutile Oxide Surfaces. *ChemCatChem*, **2012**, 4, 1856-1861	5.2	11
32	Universal transition state scaling relations for (de)hydrogenation over transition metals. *Physical Chemistry Chemical Physics*, **2011**, 13, 20760-5	3.6	295
31	Scaling relationships for adsorption energies of C2 hydrocarbons on transition metal surfaces. *Chemical Engineering Science*, **2011**, 66, 6318-6323	4.4	93
30	Density functional theory in surface chemistry and catalysis. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 937-43	11.5	1141
29	Universal Brønsted-Evans-Polanyi Relations for C□, C□, C□, N□, N□, and O□ Dissociation Reactions. *Catalysis Letters*, **2011**, 141, 370-373	2.8	215
28	Descriptor-Based Analysis Applied to HCN Synthesis from NH3 and CH4. *Angewandte Chemie*, **2011**, 123, 4697-4701	3.6	11
27	Descriptor-based analysis applied to HCN synthesis from NH3 and CH4. *Angewandte Chemie - International Edition*, **2011**, 50, 4601-5	16.4	68
26	On the behavior of Brønsted-Evans-Polanyi relations for transition metal oxides. *Journal of Chemical Physics*, **2011**, 134, 244509	3.9	108
25	Structure effects on the energetics of the electrochemical reduction of CO2 by copper surfaces. *Surface Science*, **2011**, 605, 1354-1359	1.8	368
24	Electrochemical chlorine evolution at rutile oxide (110) surfaces. *Physical Chemistry Chemical Physics*, **2010**, 12, 283-90	3.6	244
23	Volcano Relation for the Deacon Process over Transition-Metal Oxides. *ChemCatChem*, **2010**, 2, 98-102	5.2	48
22	How copper catalyzes the electroreduction of carbon dioxide into hydrocarbon fuels. *Energy and Environmental Science*, **2010**, 3, 1311	35.4	1861
21	Identification of non-precious metal alloy catalysts for selective hydrogenation of acetylene. *Science*, **2008**, 320, 1320-2	33.3	795
20	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, 644-52	4.8	70
19	On the role of surface modifications of palladium catalysts in the selective hydrogenation of acetylene. *Angewandte Chemie - International Edition*, **2008**, 47, 9299-302	16.4	197

18	On the Role of Surface Modifications of Palladium Catalysts in the Selective Hydrogenation of Acetylene. *Angewandte Chemie*, **2008**, 120, 9439-9442	3.6	33
17	Scaling properties of adsorption energies for hydrogen-containing molecules on transition-metal surfaces. *Physical Review Letters*, **2007**, 99, 016105	7.4	1009
16	Spectroscopic Comparison of Dinuclear Ti+ and Ti2+ 1:1 Dinitrogen Complexes with Cp*/Pentafulvene and Amine/Amide Ligation: Moderate versus Strong Activation of N2. *European Journal of Inorganic Chemistry*, **2006**, 2006, 291-297	2.3	19
15	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, 1278-91	3.5	111
14	N-N splitting of a functionalized mu-eta1:eta2 coordinated N2 ligand leading to a micro-nitrido micro-imido core: mechanistic insight from DFT. *Dalton Transactions*, **2006**, 1137-40	4.3	15
13	Combined In Situ EDXRD/EXAFS Investigation of the Crystal Growth of [Co(C6H18N4)][Sb2S4] under Solvothermal Conditions: Two Different Reaction Pathways Leading to the Same Product. *Chemistry of Materials*, **2006**, 18, 1196-1205	9.6	61
12	Orbital interactions in Fe(II)/Co(III) heterobimetallocenes: single versus double bridge. *Inorganic Chemistry*, **2006**, 45, 2531-42	5.1	13
11	Vibrational and electronic structure of the dinuclear bis(mu-nitrido) vanadium(v) complex [V(N{N"}2)(mu-N)]2: spectroscopic properties of the M2(mu-N)2 diamond core. *Dalton Transactions*, **2005**, 1052-7	4.3	16
10	Reduction pathway of end-on terminally coordinated dinitrogen. V. N-N bond cleavage in Mo/W hydrazidium complexes with diphosphine coligands. Comparison with triamidoamine systems. *Inorganic Chemistry*, **2005**, 44, 3031-45	5.1	49
9	Dismutation of a Molybdenum(IV) Acetonitrile NNH2Complex to a Molybdenum(IV) Ethylimido Complex + N2: Mechanistic Implications on the Protonation of Coordinated Nitriles at the Carbon Atom. *Organometallics*, **2005**, 24, 5393-5406	3.8	11
8	Energetics and mechanism of a room-temperature catalytic process for ammonia synthesis (Schrock cycle): comparison with biological nitrogen fixation. *Angewandte Chemie - International Edition*, **2005**, 44, 5639-42	16.4	134
7	Energetik und Mechanismus einer katalytischen Ammoniaksynthese bei Raumtemperatur (Schrock-Zyklus); Vergleich mit der biologischen Stickstoff-Fixierung. *Angewandte Chemie*, **2005**, 117, 5783-5787	3.6	50
6	Lewis adducts of the side-on end-on dinitrogen-bridged complex [{(NPN)Ta}2(mu-H)2(mu-eta 1:eta 2-N2)] with AlMe3, GaMe3, and B(C6F5)3: synthesis, structure, and spectroscopic properties. *Chemistry - A European Journal*, **2005**, 11, 604-18	4.8	39
5	[Ni(C4H13N3)2]3(Sb3S6)2: The First Structure Containing Isolated Heterocyclic [Sb3S6]3 Anions. *European Journal of Inorganic Chemistry*, **2004**, 2004, 2553-2556	2.3	51
4	Application of a universal force field to mixed Fe/Mo-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/Se. *Inorganic Chemistry*, **2004**, 43, 5003-10	5.1	15
3	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: correlations to electronic structure and reactivity. *Journal of the American Chemical Society*, **2004**, 126, 280-90	16.4	40
2	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, 520-30	4.8	29
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