Philippe Sautet

List of Publications by Year
in descending order

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407 papers	25,449 citations	5248 83 h-index	11030 137 g-index
423 all docs	423 docs citations	423 times ranked	18540 citing authors

#	Article	IF	Citations
1	Revisiting the Link between Magnetic Properties and Chemisorption at Graphene Nanoribbon Zigzag Edge. Journal of Chemical Physics, 2022, 156, 044706.	1.2	1
2	Toward benchmarking theoretical computations of elementary rate constants on catalytic surfaces: formate decomposition on Au and Cu. Chemical Science, 2022, 13, 804-815.	3.7	3
3	Interpreting the Operando X-ray Absorption Near-Edge Structure of Supported Cu and CuPd Clusters in Conditions of Oxidative Dehydrogenation of Propane: Dynamic Changes in Composition and Size. Journal of Physical Chemistry C, 2022, 126, 1972-1981.	1.5	3
4	Decoding reactive structures in dilute alloy catalysts. Nature Communications, 2022, 13, 832.	5.8	35
5	Reaction product-driven restructuring and assisted stabilization of a highly dispersed Rh-on-ceria catalyst. Nature Catalysis, 2022, 5, 119-127.	16.1	46
6	Dilute Alloys Based on Au, Ag, or Cu for Efficient Catalysis: From Synthesis to Active Sites. Chemical Reviews, 2022, 122, 8758-8808.	23.0	50
7	Oxidation Dynamics of Supported Catalytic Cu Clusters: Coupling to Fluxionality. ACS Catalysis, 2022, 12, 818-827.	5.5	7
8	Modeling Electrochemical Processes with Grand Canonical Treatment of Many-Body Perturbation Theory. Journal of Physical Chemistry Letters, 2022, 13, 6079-6084.	2.1	8
9	Impact of Organic Templates on the Selective Formation of Zeolite Oligomers. Angewandte Chemie - International Edition, 2021, 60, 7111-7116.	7.2	7
10	Impact of Organic Templates on the Selective Formation of Zeolite Oligomers. Angewandte Chemie, 2021, 133, 7187-7192.	1.6	9
11	Observing Singleâ€Atom Catalytic Sites During Reactions with Electrospray Ionization Mass Spectrometry. Angewandte Chemie, 2021, 133, 4814-4823.	1.6	11
12	Observing Singleâ€Atom Catalytic Sites During Reactions with Electrospray Ionization Mass Spectrometry. Angewandte Chemie - International Edition, 2021, 60, 4764-4773.	7.2	38
13	NanoCluster heterogeneous catalysts: Insights from theory. , 2021, , .		0
14	Global Activity Search Uncovers Reaction Induced Concomitant Catalyst Restructuring for Alkane Dissociation on Model Pt Catalysts. ACS Catalysis, 2021, 11, 1877-1885.	5.5	26
15	Highly dispersed Pt atoms and clusters on hydroxylated indium tin oxide: a view from first-principles calculations. Journal of Materials Chemistry A, 2021, 9, 15724-15733.	5.2	8
16	RÃ¼cktitelbild: Impact of Organic Templates on the Selective Formation of Zeolite Oligomers (Angew.) Tj ETQq0 0 0 rgBT /Overlock 10	1.6	0
17	Structure-sensitive scaling relations among carbon-containing species and their possible impact on CO2 electroreduction. Journal of Catalysis, 2021, 395, 136-142.	3.1	6
18	Atomic Environments in N-Containing Graphitic Carbon Probed by First-Principles Calculations and Solid-State Nuclear Magnetic Resonance. Journal of Physical Chemistry C, 2021, 125, 8779-8787.	1.5	4

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19	Formation of a Tiâ€“Cu(111) single atom alloy: Structure and CO binding. Journal of Chemical Physics, 2021, 154, 234703.	1.2	13
20	Entropic Control of HD Exchange Rates over Dilute Pd-in-Au Alloy Nanoparticle Catalysts. ACS Catalysis, 2021, 11, 6971-6981.	5.5	25
21	Identification of active catalysts for the acceptorless dehydrogenation of alcohols to carbonyls. Nature Communications, 2021, 12, 5100.	5.8	21
22	Thermodynamics of Atomic Layer Etching Chemistry on Copper and Nickel Surfaces from First Principles. Chemistry of Materials, 2021, 33, 6774-6786.	3.2	3
23	Active Site Fluxional Restructuring as a New Paradigm in Triggering Reaction Activity for Nanocluster Catalysis. Accounts of Chemical Research, 2021, 54, 3841-3849.	7.6	17
24	What does graphitic carbon nitride really look like?. Physical Chemistry Chemical Physics, 2021, 23, 2853-2859.	1.3	12
25	Avoiding dendrite formation by confining lithium deposition underneath Liâ€“Sn coatings. Journal of Materials Research, 2021, 36, 797-811.	1.2	4
26	Thermokinetic and Spectroscopic Mapping of Carbon Monoxide Adsorption on Highly Dispersed Pt/Î³-Al₂O₃. ACS Catalysis, 2021, 11, 13280-13293.	5.5	17
27	CO organization at ambient pressure on stepped Pt surfaces: first principles modeling accelerated by neural networks. Chemical Science, 2021, 12, 15543-15555.	3.7	8
28	Diffusion Barriers for Carbon Monoxide on the Cu(001) Surface Using Many-Body Perturbation Theory and Various Density Functionals. Journal of Chemical Theory and Computation, 2021, 17, 7862-7872.	2.3	10
29	Mechanistic and Electronic Insights into a Working NiAu Single-Atom Alloy Ethanol Dehydrogenation Catalyst. Journal of the American Chemical Society, 2021, 143, 21567-21579.	6.6	28
30	Global Optimization of Adsorbate Covered Supported Cluster Catalysts: The Case of Pt₇H₁₀CH₃ on Î±â€Al₂O₃. ChemCatChem, 2020, 12, 762-770.	1.8	11
31	Achieving High Selectivity for Alkyne Hydrogenation at High Conversions with Compositionally Optimized PdAu Nanoparticle Catalysts in Raspberry Colloid-Templated SiO₂. ACS Catalysis, 2020, 10, 441-450.	5.5	61
32	Effect of Frustrated Rotations on the Pre-Exponential Factor for Unimolecular Reactions on Surfaces: A Case Study of Alkoxy Dehydrogenation. Journal of Physical Chemistry C, 2020, 124, 1429-1437.	1.5	10
33	Mononuclear Fe in N-doped carbon: computational elucidation of active sites for electrochemical oxygen reduction and oxygen evolution reactions. Catalysis Science and Technology, 2020, 10, 1006-1014.	2.1	34
34	Insights into Copper Sulfide Formation from Cu and S K edge XAS and DFT studies. Inorganic Chemistry, 2020, 59, 15276-15288.	1.9	8
35	Stabilizing Oxidative Dehydrogenation Active Sites at High Temperature with Steam: ZnFe₂O₄-Catalyzed Oxidative Dehydrogenation of 1-Butene to 1,3-Butadiene. ACS Catalysis, 2020, 10, 12888-12897.	5.5	11
36	Dual redox mediators accelerate the electrochemical kinetics of lithium-sulfur batteries. Nature Communications, 2020, 11, 5215.	5.8	113

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37	Guidelines to Achieving High Selectivity for the Hydrogenation of Î±,Î²-Unsaturated Aldehydes with Bimetallic and Dilute Alloy Catalysts: A Review. Chemical Reviews, 2020, 120, 12834-12872.	23.0	136
38	Optimal Packing of CO at a High Coverage on Pt(100) and Pt(111) Surfaces. ACS Catalysis, 2020, 10, 9533-9544.	5.5	21
39	Hydrogen Evolution on Restructured B-Rich WB: Metastable Surface States and Isolated Active Sites. ACS Catalysis, 2020, 10, 13867-13877.	5.5	20
40	Atomic layer etching of metals with anisotropy, specificity, and selectivity. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2020, 38, .	0.9	8
41	Evolution of Metastable Structures at Bimetallic Surfaces from Microscopy and Machine-Learning Molecular Dynamics. Journal of the American Chemical Society, 2020, 142, 15907-15916.	6.6	47
42	Facilitating hydrogen atom migration via a dense phase on palladium islands to a surrounding silver surface. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 22657-22664.	3.3	26
43	A Perspective on interfacial engineering of lithium metal anodes and beyond. Applied Physics Letters, 2020, 117, .	1.5	18
44	A fundamental look at electrocatalytic sulfur reduction reaction. Nature Catalysis, 2020, 3, 762-770.	16.1	455
45	Facile Decomposition of Organophosphonates by Dual Lewis Sites on a Fe₃O₄(111) Film. Journal of Physical Chemistry C, 2020, 124, 12432-12441.	1.5	13
46	Stoichiometry-controllable optical defects in Cu_xIn_{2â^'x}S_y quantum dots for energy harvesting. Journal of Materials Chemistry A, 2020, 8, 12556-12565.	5.2	8
47	Excellence versus Diversity? Not an Either/Or Choice. ACS Catalysis, 2020, 10, 7310-7311.	5.5	4
48	Reagent-Triggered Isomerization of Fluxional Cluster Catalyst via Dynamic Coupling. Journal of Physical Chemistry Letters, 2020, 11, 3089-3094.	2.1	19
49	CO Oxidation Mechanisms on CoO_x-Pt Thin Films. Journal of the American Chemical Society, 2020, 142, 8312-8322.	6.6	39
50	Interpreting the Operando XANES of Surface-Supported Subnanometer Clusters: When Fluxionality, Oxidation State, and Size Effect Fight. Journal of Physical Chemistry C, 2020, 124, 10057-10066.	1.5	24
51	Structural Rearrangements of Subnanometer Cu Oxide Clusters Govern Catalytic Oxidation. ACS Catalysis, 2020, 10, 5309-5317.	5.5	36
52	Tuning reactivity layer-by-layer: formic acid activation on Ag/Pd(111). Chemical Science, 2020, 11, 6492-6499.	3.7	7
53	Understanding the influence of the composition of the Ag Pd catalysts on the selective formic acid decomposition and subsequent levulinic acid hydrogenation. International Journal of Hydrogen Energy, 2020, 45, 17339-17353.	3.8	29
54	Rational design of selective metal catalysts for alcohol amination with ammonia. Nature Catalysis, 2019, 2, 773-779.	16.1	70

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55	Reactivity of shape-controlled crystals and metadynamics simulations locate the weak spots of alumina in water. Nature Communications, 2019, 10, 3139.	5.8	42
56	Evaluating Thermal Corrections for Adsorption Processes at the Metal/Gas Interface. Journal of Physical Chemistry C, 2019, 123, 28828-28835.	1.5	17
57	Toward Fast and Reliable Potential Energy Surfaces for Metallic Pt Clusters by Hierarchical Delta Neural Networks. Journal of Chemical Theory and Computation, 2019, 15, 5614-5627.	2.3	34
58	Effects of Morphology and Surface Properties of Copper Oxide on the Removal of Hydrogen Sulfide from Gaseous Streams. Industrial & Engineering Chemistry Research, 2019, 58, 18836-18847.	1.8	21
59	Surface Structure of Co₃O₄ (111) under Reactive Gas-Phase Environments. ACS Catalysis, 2019, 9, 6380-6392.	5.5	27
60	Automated Detection and Characterization of Surface Restructuring Events in Bimetallic Catalysts. Journal of Physical Chemistry C, 2019, 123, 16332-16344.	1.5	10
61	Single-atom tailoring of platinum nanocatalysts for high-performance multifunctional electrocatalysis. Nature Catalysis, 2019, 2, 495-503.	16.1	464
62	The Pressure Gap for Thiols: Methanethiol Self-Assembly on Au(111) from Vacuum to 1 bar. Journal of Physical Chemistry C, 2019, 123, 12382-12389.	1.5	7
63	Atomically Dispersed Pt₁â€“Polyoxometalate Catalysts: How Does Metalâ€“Support Interaction Affect Stability and Hydrogenation Activity?. Journal of the American Chemical Society, 2019, 141, 8185-8197.	6.6	147
64	Water on Oxide Surfaces: A Triaqua Surface Coordination Complex on Co₃O₄(111). Journal of the American Chemical Society, 2019, 141, 5623-5627.	6.6	18
65	Theory and experiments join forces to characterize the electrocatalytic interface. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 7611-7613.	3.3	5
66	Affordable Estimation of Solvation Contributions to the Adsorption Energies of Oxygenates on Metal Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 5578-5582.	1.5	54
67	Heterogeneity in Local Chemical Bonding Explains Spectral Broadening in Quantum Dots with Cu Impurities. Journal of Physical Chemistry C, 2019, 123, 5705-5713.	1.5	12
68	Pt8 cluster on alumina under a pressure of hydrogen: Support-dependent reconstruction from first-principles global optimization. Journal of Chemical Physics, 2019, 151, 194703.	1.2	34
69	Rh single atoms on TiO2 dynamically respond to reaction conditions by adapting their site. Nature Communications, 2019, 10, 4488.	5.8	191
70	Dehydrogenation mechanisms of methyl-cyclohexane on Î³-Al2O3 supported Pt13: Impact of cluster ductility. Journal of Catalysis, 2019, 370, 118-129.	3.1	47
71	Unravelling the Metastable Nature of the Single Site Tungsten Hydride Metathesis Catalyst Supported on Î³-Alumina from First Principles. Journal of Physical Chemistry C, 2019, 123, 1226-1234.	1.5	2
72	Dynamics of Surface Alloys: Rearrangement of Pd/Ag(111) Induced by CO and O₂. Journal of Physical Chemistry C, 2019, 123, 8312-8323.	1.5	75

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73	Computational screening for selective catalysts: Cleaving the C C bond during ethanol electro-oxidation reaction. Electrochimica Acta, 2018, 274, 274-278.	2.6	26
74	Acidâ€“Base Control of Valency within Carboranedithiol Self-Assembled Monolayers: Molecules Do the Can-Can. ACS Nano, 2018, 12, 2211-2221.	7.3	23
75	Metastable Structures in Cluster Catalysis from First-Principles: Structural Ensemble in Reaction Conditions and Metastability Triggered Reactivity. Journal of the American Chemical Society, 2018, 140, 2812-2820.	6.6	131
76	Evaluating the Risk of Câ€“C Bond Formation during Selective Hydrogenation of Acetylene on Palladium. ACS Catalysis, 2018, 8, 1662-1671.	5.5	65
77	Force Field for Water over Pt(111): Development, Assessment, and Comparison. Journal of Chemical Theory and Computation, 2018, 14, 3238-3251.	2.3	38
78	Structuration and Dynamics of Interfacial Liquid Water at Hydrated Î³-Alumina Determined by ab Initio Molecular Simulations: Implications for Nanoparticle Stability. ACS Applied Nano Materials, 2018, 1, 191-199.	2.4	37
79	Direct n-octanol amination by ammonia on supported Ni and Pd catalysts: activity is enhanced by â€œspectatorâ€•ammonia adsorbates. Catalysis Science and Technology, 2018, 8, 611-621.	2.1	26
80	Trends and Control in the Nitridation of Transition-Metal Surfaces. ACS Catalysis, 2018, 8, 63-68.	5.5	19
81	Theoretical Treatment of Surfaces in Equilibrium with Gases. , 2018, , 684-698.		1
82	Unraveling the Role of Base and Catalyst Polarization in Alcohol Oxidation on Au and Pt in Water. ACS Catalysis, 2018, 8, 11716-11721.	5.5	31
83	DFT investigations for the catalytic reaction mechanism of methane combustion occurring on Pd(<scp>ii</scp>)/Al-MCM-41. Physical Chemistry Chemical Physics, 2018, 20, 25377-25386.	1.3	8
84	Contribution of electrolyte in nanoscale electrolysis of pure and buffered water by particulate photocatalysis. Sustainable Energy and Fuels, 2018, 2, 2044-2052.	2.5	18
85	Câ€“H Activation and Proton Transfer Initiate Alkene Metathesis Activity of the Tungsten(IV)â€“Oxo Complex. Journal of the American Chemical Society, 2018, 140, 11395-11401.	6.6	21
86	Shining Light on Carbon Nitrides: Leveraging Temperature To Understand Optical Gap Variations. Chemistry of Materials, 2018, 30, 4253-4262.	3.2	28
87	Acetylene Adsorption on Pdâ€“Ag Alloys: Evidence for Limited Island Formation and Strong Reverse Segregation from Monte Carlo Simulations. Journal of Physical Chemistry C, 2018, 122, 15456-15463.	1.5	35
88	Direct Amination of Alcohols Catalyzed by Aluminum Triflate: Anâ€‰Experimental and Computational Study. Chemistry - A European Journal, 2018, 24, 14146-14153.	1.7	13
89	Supported goldâ€“nickel nano-alloy as a highly efficient catalyst in levulinic acid hydrogenation with formic acid as an internal hydrogen source. Catalysis Science and Technology, 2018, 8, 4318-4331.	2.1	51
90	Key Role of Anionic Doping for H₂ Production from Formic Acid on Pd(111). ACS Catalysis, 2017, 7, 1955-1959.	5.5	72

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91	Challenges in calculating the bandgap of triazine-based carbon nitride structures. Journal of Materials Chemistry A, 2017, 5, 5115-5122.	5.2	34
92	Photophysical Properties of SrTaO₂N Thin Films and Influence of Anion Ordering: A Joint Theoretical and Experimental Investigation. Chemistry of Materials, 2017, 29, 3989-3998.	3.2	37
93	Adsorption and Decomposition of a Lignin Î²-O-4 Linkage Model, 2-Phenoxyethanol, on Pt(111): Combination of Experiments and First-Principles Calculations. Journal of Physical Chemistry C, 2017, 121, 9889-9900.	1.5	16
94	Isosorbide telechelic bio-based oligomers. Journal of Polymer Science Part A, 2017, 55, 2178-2189.	2.5	4
95	Understanding the influence of hydrogen pressure on the enantioselectivity of hydrogenation: A combined theory-experiment approach. Journal of Organometallic Chemistry, 2017, 836-837, 90-99.	0.8	3
96	Why conclusions from platinum model surfaces do not necessarily lead to enhanced nanoparticle catalysts for the oxygen reduction reaction. Chemical Science, 2017, 8, 2283-2289.	3.7	173
97	Coadsorption of Butadiene and Hydrogen on the (111) Surfaces of Pt and Pt2Sn Surface Alloy: Understanding the Cohabitation from First-Principles Calculations. Journal of Physical Chemistry C, 2017, 121, 25152-25163.	1.5	14
98	Bismuth Silver Oxysulfide for Photoconversion Applications: Structural and Optoelectronic Properties. Chemistry of Materials, 2017, 29, 8679-8689.	3.2	28
99	Group Additivity for Aqueous Phase Thermochemical Properties of Alcohols on Pt(111). Journal of Physical Chemistry C, 2017, 121, 21510-21519.	1.5	27
100	Molecular mechanics models for the image charge, a comment on â€œincluding image charge effects in the molecular dynamics simulations of molecules on metal surfacesâ€• Journal of Computational Chemistry, 2017, 38, 2127-2129.	1.5	9
101	A machine learning approach to graph-theoretical cluster expansions of the energy of adsorbate layers. Journal of Chemical Physics, 2017, 147, 054106.	1.2	31
102	Developing a Descriptor-Based Approach for CO and NO Adsorption Strength to Transition Metal Sites in Zeolites. Chemistry of Materials, 2017, 29, 6434-6444.	3.2	34
103	Oxidation of Methane to Methanol over Single Site Palladium Oxide Species on Silica: A Mechanistic view from DFT. Journal of Physical Chemistry A, 2017, 121, 5500-5508.	1.1	18
104	Enhanced Kinetics of Hole Transfer and Electrocatalysis during Photocatalytic Oxygen Evolution by Cocatalyst Tuning. ACS Catalysis, 2016, 6, 4117-4126.	5.5	48
105	Controlling the Adsorption of Aromatic Compounds on Pt(111) with Oxygenate Substituents: From DFT to Simple Molecular Descriptors. Journal of Physical Chemistry Letters, 2016, 7, 2074-2079.	2.1	23
106	Role of Tricoordinate Al Sites in CH₃ReO₃/Al₂O₃ Olefin Metathesis Catalysts. Journal of the American Chemical Society, 2016, 138, 6774-6785.	6.6	42
107	The mechanism of the initial step of germanosilicate formation in solution: a first-principles molecular dynamics study. Physical Chemistry Chemical Physics, 2016, 18, 14419-14425.	1.3	7
108	DFT Perspective on the Thermochemistry of Carbon Nitride Synthesis. Journal of Physical Chemistry C, 2016, 120, 24542-24550.	1.5	21

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109	How Should Iron and Titanium be Combined in Oxides to Improve Photoelectrochemical Properties?. Journal of Physical Chemistry C, 2016, 120, 24521-24532.	1.5	35
110	Capturing Solvation Effects at a Liquid/Nanoparticle Interface by Ab Initio Molecular Dynamics: Pt₂₀₁ Immersed in Water. Small, 2016, 12, 5312-5319.	5.2	25
111	Characterization and charge transfer properties of organic BODIPY dyes integrated in TiO₂nanotube based dye-sensitized solar cells. RSC Advances, 2016, 6, 91529-91540.	1.7	17
112	Structural Characterization of the EtOHâ€“TiCl₄â€“MgCl₂ Zieglerâ€“Natta Precatalyst. Journal of Physical Chemistry C, 2016, 120, 18075-18087.	1.5	28
113	Computationally Exploring Confinement Effects in the Methane-to-Methanol Conversion Over Iron-Oxo Centers in Zeolites. ACS Catalysis, 2016, 6, 8404-8409.	5.5	83
114	C₂H₂-Induced Surface Restructuring of Pdâ€“Ag Catalysts: Insights from Theoretical Modeling. Journal of Physical Chemistry C, 2016, 120, 26320-26327.	1.5	26
115	Decomposition Mechanism of Anisole on Pt(111): Combining Single-Crystal Experiments and First-Principles Calculations. ACS Catalysis, 2016, 6, 8166-8178.	5.5	34
116	Solvation free energies for periodic surfaces: comparison of implicit and explicit solvation models. Physical Chemistry Chemical Physics, 2016, 18, 31850-31861.	1.3	80
117	How Does the Surface Structure of Ptâ€“Ni Alloys Control Water and Hydrogen Peroxide Formation?. ACS Catalysis, 2016, 6, 5641-5650.	5.5	9
118	Towards more accurate prediction of activation energies for polyalcohol dehydrogenation on transition metal catalysts in water. Catalysis Science and Technology, 2016, 6, 6615-6624.	2.1	31
119	Ethanol Electro-oxidation on Palladium Revisited Using Polarization Modulation Infrared Reflection Absorption Spectroscopy (PM-IRRAS) and Density Functional Theory (DFT): Why Is It Difficult To Break the Câ€“C Bond?. ACS Catalysis, 2016, 6, 4894-4906.	5.5	109
120	Performance and degradation of Proton Exchange Membrane Fuel Cells: State of the art in modeling from atomistic to system scale. Journal of Power Sources, 2016, 304, 207-233.	4.0	180
121	The impact of finite temperature on the coordination of Cu cations in the zeolite SSZ-13. Catalysis Today, 2016, 267, 41-46.	2.2	33
122	Electro-carboxylation of butadiene and ethene over Pt and Ni catalysts. Journal of Catalysis, 2016, 343, 240-247.	3.1	31
123	Assessing a First-Principles Model of an Electrochemical Interface by Comparison with Experiment. Journal of Physical Chemistry C, 2016, 120, 5619-5623.	1.5	78
124	Ru catalysts for levulinic acid hydrogenation with formic acid as a hydrogen source. Green Chemistry, 2016, 18, 2014-2028.	4.6	126
125	Verursacht Dynamik das komplexe Infrarotspektrum von NO an Kupfer(II)â€Zentren in Zeolithen?. Angewandte Chemie, 2015, 127, 7910-7915.	1.6	8
126	Can Dynamics Be Responsible for the Complex Multipeak Infrared Spectra of NO Adsorbed to Copper(II) Sites in Zeolites?. Angewandte Chemie - International Edition, 2015, 54, 7799-7804.	7.2	39

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127	Modeling the HCOOH/CO₂ Electrocatalytic Reaction: When Details Are Key. ChemPhysChem, 2015, 16, 2307-2311.	1.0	44
128	In Silico Screening of Iron-Oxo Catalysts for CH Bond Cleavage. ACS Catalysis, 2015, 5, 2490-2499.	5.5	35
129	Trade-Off between Accuracy and Universality in Linear Energy Relations for Alcohol Dehydrogenation on Transition Metals. Journal of Physical Chemistry C, 2015, 119, 12988-12998.	1.5	46
130	Surface ReO_x Sites on Al₂O₃ and Their Molecular Structureâ€“Reactivity Relationships for Olefin Metathesis. ACS Catalysis, 2015, 5, 1432-1444.	5.5	64
131	Scrutinizing individual CoTPP molecule adsorbed on coinage metal surfaces from the interplay of STM experiment and theory. Surface Science, 2015, 635, 108-114.	0.8	12
132	Titaniaâ€Supported Catalysts for Levulinic Acid Hydrogenation: Influence of Support and its Impact on Î³â€Valerolactone Yield. ChemSusChem, 2015, 8, 1538-1547.	3.6	85
133	Carbonâ€“Carbon Bond Formation by Activation of CH₃F on Alumina. Journal of Physical Chemistry C, 2015, 119, 7156-7163.	1.5	28
134	ACS Catalysis Appoints Takashi Ooi as Associate Editor and Posts Virtual Special Issue on Theory and Computation in Catalysis. ACS Catalysis, 2015, 5, 3027-3027.	5.5	1
135	Impacts of electrode potentials and solvents on the electroreduction of CO₂: a comparison of theoretical approaches. Physical Chemistry Chemical Physics, 2015, 17, 13949-13963.	1.3	90
136	Coverage-dependent thermodynamic analysis of the formation of water and hydrogen peroxide on a platinum model catalyst. Physical Chemistry Chemical Physics, 2015, 17, 11392-11400.	1.3	20
137	Electronic structure and photocatalytic activity of wurtzite Cuâ€“Gaâ€“S nanocrystals and their Zn substitution. Journal of Materials Chemistry A, 2015, 3, 8896-8904.	5.2	33
138	A Salute to My Colleague Yves Chauvin, 1930â€“2015. ACS Catalysis, 2015, 5, 2115-2115.	5.5	1
139	Introducing structural sensitivity into adsorptionâ€“energy scaling relations by means of coordination numbers. Nature Chemistry, 2015, 7, 403-410.	6.6	600
140	Restoring the Co Magnetic Moments at Interfacial Co-Porphyrin Arrays by Site-Selective Uptake of Iron. ACS Nano, 2015, 9, 3605-3616.	7.3	17
141	Grafting trimethylaluminum and its halogen derivatives on silica: general trends for²⁷Al SS-NMR response from first principles calculations. Physical Chemistry Chemical Physics, 2015, 17, 26937-26945.	1.3	10
142	Relationship between Carbon Nitride Structure and Exciton Binding Energies: A DFT Perspective. Journal of Physical Chemistry C, 2015, 119, 25188-25196.	1.5	104
143	Molecular adsorption at Pt(111). How accurate are DFT functionals?. Physical Chemistry Chemical Physics, 2015, 17, 28921-28930.	1.3	210
144	Finding optimal surface sites on heterogeneous catalysts by counting nearest neighbors. Science, 2015, 350, 185-189.	6.0	725

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145	Cooperativity between Al Sites Promotes Hydrogen Transfer and Carbonâ€“Carbon Bond Formation upon Dimethyl Ether Activation on Alumina. ACS Central Science, 2015, 1, 313-319.	5.3	92
146	Dendritic Tip-on Polytriazine-Based Carbon Nitride Photocatalyst with High Hydrogen Evolution Activity. Chemistry of Materials, 2015, 27, 8237-8247.	3.2	140
147	Interplay between Reaction Mechanism and Hydroxyl Species for Water Formation on Pt(111). ACS Catalysis, 2015, 5, 1068-1077.	5.5	24
148	Electronic properties of PbX₃CH₃NH₃ (X = Cl, Br, I) compounds for photovoltaic and photocatalytic applications. Physical Chemistry Chemical Physics, 2015, 17, 2199-2209.	1.3	52
149	Modeling the adsorption of short alkanes in the zeolite SSZ-13 using â€œvan der Waalsâ€•DFT exchange correlation functionals: Understanding the advantages and limitations of such functionals. Journal of Chemical Physics, 2014, 140, 154105.	1.2	21
150	Chlorodiethylaluminum supported on silica: A dinuclear aluminum surface species with bridging Î¼2-Cl-ligand as a highly efficient co-catalyst for the Ni-catalyzed dimerization of ethene. Journal of Catalysis, 2014, 313, 46-54.	3.1	43
151	Formation of Acrylates from Ethylene and CO₂ on Ni Complexes: A Mechanistic Viewpoint from a Hybrid DFT Approach. Organometallics, 2014, 33, 6369-6380.	1.1	36
152	Tuning the properties of visible-light-responsive tantalum (oxy)nitride photocatalysts by non-stoichiometric compositions: a first-principles viewpoint. Physical Chemistry Chemical Physics, 2014, 16, 20548-20560.	1.3	86
153	Control of the anisotropic shape of cobalt nanorods in the liquid phase: from experiment to theoryâ€¦ and back. Nanoscale, 2014, 6, 2682.	2.8	39
154	Visibility of Al Surface Sites of Î³-Alumina: A Combined Computational and Experimental Point of View. Journal of Physical Chemistry C, 2014, 118, 15292-15299.	1.5	97
155	How Surface Hydroxyls Enhance MgO Reactivity in Basic Catalysis: The Case of Methylbutynol Conversion. ACS Catalysis, 2014, 4, 4004-4014.	5.5	34
156	Linear Energy Relations As Predictive Tools for Polyalcohol Catalytic Reactivity. ACS Catalysis, 2014, 4, 464-468.	5.5	41
157	Critical Role of the Semiconductorâ€“Electrolyte Interface in Photocatalytic Performance for Water-Splitting Reactions Using Ta₃N₅ Particles. Chemistry of Materials, 2014, 26, 4812-4825.	3.2	98
158	Understanding Adsorption-Induced Effects on Platinum Nanoparticles: An Energy-Decomposition Analysis. Journal of Physical Chemistry Letters, 2014, 5, 3120-3124.	2.1	37
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