Philippe Sautet

List of Publications by Year
in descending order

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407 papers	25,449 citations	5268 83 h-index	11052 137 g-index
423 all docs	423 docs citations	423 times ranked	18540 citing authors

#	Article	IF	Citations
1	Use of DFT to achieve a rational understanding of acid?basic properties of ?-alumina surfaces. Journal of Catalysis, 2004, 226, 54-68.	6.2	880
2	Finding optimal surface sites on heterogeneous catalysts by counting nearest neighbors. Science, 2015, 350, 185-189.	12.6	725
3	Introducing structural sensitivity into adsorptionâ€“energy scaling relations by means of coordination numbers. Nature Chemistry, 2015, 7, 403-410.	13.6	600
4	Hydroxyl Groups on Î³-Alumina Surfaces: A DFT Study. Journal of Catalysis, 2002, 211, 1-5.	6.2	485
5	Single-atom tailoring of platinum nanocatalysts for high-performance multifunctional electrocatalysis. Nature Catalysis, 2019, 2, 495-503.	34.4	464
6	A fundamental look at electrocatalytic sulfur reduction reaction. Nature Catalysis, 2020, 3, 762-770.	34.4	455
7	Competitive Cî—»C and Cî—»O Adsorption of Î±-Î²-Unsaturated Aldehydes on Pt and Pd Surfaces in Relation with the Selectivity of Hydrogenation Reactions: A Theoretical Approach. Journal of Catalysis, 1995, 152, 217-236.	6.2	446
8	Stability and Reactivity of Ïµâˆ’Ï‡âˆ’Î¸ Iron Carbide Catalyst Phases in Fischerâˆ’Tropsch Synthesis: Controlling Î¼_C. Journal of the American Chemical Society, 2010, 132, 14928-14941.	13.7	426
9	Fast Prediction of Adsorption Properties for Platinum Nanocatalysts with Generalized Coordination Numbers. Angewandte Chemie - International Edition, 2014, 53, 8316-8319.	13.8	366
10	Hydroxyl Groups on Î³-Alumina Surfaces: A DFT Study. Journal of Catalysis, 2002, 211, 1-5.	6.2	364
11	Î³-Alumina: The Essential and Unexpected Role of Water for the Structure, Stability, and Reactivity of â€œDefectâ€•Sites. Journal of the American Chemical Society, 2012, 134, 14430-14449.	13.7	308
12	Calculation of the benzene on rhodium STM images. Chemical Physics Letters, 1991, 185, 23-30.	2.6	274
13	Structure and Stability of Aluminum Hydroxides:Â A Theoretical Study. Journal of Physical Chemistry B, 2002, 106, 5155-5162.	2.6	241
14	Semiconductors Used in Photovoltaic and Photocatalytic Devices: Assessing Fundamental Properties from DFT. Journal of Physical Chemistry C, 2014, 118, 5997-6008.	3.1	239
15	Significance of single-electron energies for the description of CO on Pt(111). Physical Review B, 2003, 68, .	3.2	225
16	How to Control the Selectivity of Palladiumâ€based Catalysts in Hydrogenation Reactions: The Role of Subsurface Chemistry. ChemCatChem, 2012, 4, 1048-1063.	3.7	223
17	Molecular adsorption at Pt(111). How accurate are DFT functionals?. Physical Chemistry Chemical Physics, 2015, 17, 28921-28930.	2.8	210
18	Images of Adsorbates with the Scanning Tunneling Microscope:â€‰ Theoretical Approaches to the Contrast Mechanism. Chemical Reviews, 1997, 97, 1097-1116.	47.7	203

#	Article	IF	Citations
19	Hydrogen adsorption on palladium: a comparative theoretical study of different surfaces. Surface Science, 1998, 411, 123-136.	1.9	198
20	Electronic interference produced by a benzene embedded in a polyacetylene chain. Chemical Physics Letters, 1988, 153, 511-516.	2.6	195
21	Rh single atoms on TiO2 dynamically respond to reaction conditions by adapting their site. Nature Communications, 2019, 10, 4488.	12.8	191
22	Understanding Palladium Hydrogenation Catalysts: When the Nature of the Reactive Molecule Controls the Nature of the Catalyst Active Phase. Angewandte Chemie - International Edition, 2008, 47, 9274-9278.	13.8	185
23	Optimal Water Coverage on Alumina: A Key to Generate Lewis Acidâ€“Base Pairs that are Reactive Towards the Cï£¿H Bond Activation of Methane. Angewandte Chemie - International Edition, 2011, 50, 3202-3205.	13.8	184
24	Dependence of stretching frequency on surface coverage and adsorbateâ€“adsorbate interactions: a density-functional theory approach of CO on Pd (111). Surface Science, 1999, 425, 68-80.	1.9	180
25	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.	7.8	180
26	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.	7.4	173
27	Molecular and dissociative chemisorption of NO on palladium and rhodium (100) and (111) surfaces: A density-functional periodic study. Journal of Chemical Physics, 1998, 108, 6447-6457.	3.0	171
28	Role of water in metal catalyst performance for ketone hydrogenation: a joint experimental and theoretical study on levulinic acid conversion into gamma-valerolactone. Chemical Communications, 2014, 50, 12450-12453.	4.1	168
29	Electronic transmission coefficient for the single-impurity problem in the scattering-matrix approach. Physical Review B, 1988, 38, 12238-12247.	3.2	167
30	Chemisorption of Benzene on Pt(111), Pd(111), and Rh(111) Metal Surfaces:â€‰ A Structural and Vibrational Comparison from First Principles. Journal of Physical Chemistry B, 2004, 108, 5653-5665.	2.6	158
31	Site preference of CO chemisorbed on Pt(111) from density functional calculations. Surface Science, 2003, 530, 71-87.	1.9	155
32	H₂â€Induced Reconstruction of Supported Pt Clusters: Metalâ€“Support Interaction versus Surface Hydride. ChemCatChem, 2011, 3, 200-207.	3.7	152
33	Viscoelastic and electrical properties of self-assembled monolayers on gold (111) films. Langmuir, 1993, 9, 3600-3611.	3.5	149
34	Au Atoms and Dimers on the MgO(100) Surface:Â A DFT Study of Nucleation at Defects. Journal of Physical Chemistry B, 2005, 109, 8040-8048.	2.6	149
35	Efficient method for the simulation of STM images. I. Generalized Green-function formalism. Physical Review B, 1997, 56, 15885-15899.	3.2	147
36	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.	13.7	147

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37	Heterolytic Splitting of H2and CH4on Î³-Alumina as a Structural Probe for Defect Sites. Journal of Physical Chemistry B, 2006, 110, 23944-23950.	2.6	141
38	Dendritic Tip-on Polytriazine-Based Carbon Nitride Photocatalyst with High Hydrogen Evolution Activity. Chemistry of Materials, 2015, 27, 8237-8247.	6.7	140
39	Vibrational frequency and chemisorption site: a DFT-periodic study of NO on Pd (111) and Rh (111) surfaces. Chemical Physics Letters, 1998, 291, 15-23.	2.6	139
40	Modulation of catalyst particle structure upon support hydroxylation: Ab initio insights into Pd13 and Pt13/Î³-Al2O3. Journal of Catalysis, 2010, 274, 99-110.	6.2	137
41	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.	47.7	136
42	Imaging the Surface and the Interface Atoms of an Oxide Film onAg{111}by Scanning Tunneling Microscopy: Experiment and Theory. Physical Review Letters, 2000, 84, 3899-3902.	7.8	135
43	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.	13.7	131
44	Fast Prediction of Selectivity in Heterogeneous Catalysis from Extended BrÃ¸nstedâ€“Evansâ€“Polanyi Relations: A Theoretical Insight. Angewandte Chemie - International Edition, 2009, 48, 8978-8980.	13.8	126
45	Ru catalysts for levulinic acid hydrogenation with formic acid as a hydrogen source. Green Chemistry, 2016, 18, 2014-2028.	9.0	126
46	Revisiting Acido-basicity of the MgO Surface by Periodic Density Functional Theory Calculations:Â Role of Surface Topology and Ion Coordination on Water Dissociation. Journal of Physical Chemistry B, 2006, 110, 15878-15886.	2.6	125
47	Molecular Understanding of Alumina Supported Single-Site Catalysts by a Combination of Experiment and Theory. Journal of the American Chemical Society, 2006, 128, 9157-9169.	13.7	125
48	Infrared Characterization of Hydroxyl Groups on MgO:â€‰ A Periodic and Cluster Density Functional Theory Study. Journal of the American Chemical Society, 2007, 129, 6442-6452.	13.7	125
49	Chemoâ^'Regioselectivity in Heterogeneous Catalysis:Â Competitive Routes for CO and CC Hydrogenations from a Theoretical Approach. Journal of the American Chemical Society, 2006, 128, 1316-1323.	13.7	122
50	Catalysis and Surface Organometallic Chemistry: A View from Theory and Simulations. Chemical Reviews, 2010, 110, 1788-1806.	47.7	121
51	Low temperature adsorption of ethylene and butadiene on platinum and palladium surfaces: A theoretical study of the di?/? competition. Catalysis Letters, 1991, 9, 245-260.	2.6	120
52	Density-functional periodic study of the adsorption of hydrogen on a palladium (111) surface. Physical Review B, 1996, 53, 8015-8027.	3.2	120
53	Shape of molecular adsorbates in STM images: A theoretical study of benzene on Pt(111). Physical Review B, 1996, 53, 4910-4925.	3.2	118
54	A Density Functional Study of Adsorption Structures of Unsaturated Aldehydes on Pt(111): A Key Factor for Hydrogenation Selectivity. Journal of Catalysis, 2002, 211, 398-406.	6.2	118

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55	Density-Functional Study of the Adsorption and Vibration Spectra of Benzene Molecules on Pt(111). Journal of Physical Chemistry B, 2003, 107, 2995-3002.	2.6	118
56	Influence of Sn additives on the selectivity of hydrogenation of Î±-Î²-unsaturated aldehydes with Pt catalysts: a density functional study of molecular adsorption. Journal of Catalysis, 2003, 220, 115-126.	6.2	116
57	Ordered structures of CO on Pd(111) studied by STM. Surface Science, 2002, 512, 48-60.	1.9	115
58	Structure sensitivity for NO dissociation on palladium and rhodium surfaces. Journal of Catalysis, 2003, 213, 211-225.	6.2	113
59	Structures and thermodynamic phase transitions for oxygen and silver oxide phases on Ag{1 1 1}. Chemical Physics Letters, 2003, 367, 344-350.	2.6	113
60	Catalytic Hydrogenation of Unsaturated Aldehydes on Pt(111): Understanding the Selectivity from First-Principles Calculations. Angewandte Chemie - International Edition, 2005, 44, 5279-5282.	13.8	113
61	Dual redox mediators accelerate the electrochemical kinetics of lithium-sulfur batteries. Nature Communications, 2020, 11, 5215.	12.8	113
62	What Makes Copper-Exchanged SSZ-13 Zeolite Efficient at Cleaning Car Exhaust Gases?. Journal of Physical Chemistry Letters, 2013, 4, 2244-2249.	4.6	112
63	Stability of Chiral Domains Produced by Adsorption of Tartaric Acid Isomers on the Cu(110) Surface:â€‰ A Periodic Density Functional Theory Study. Journal of the American Chemical Society, 2001, 123, 6639-6648.	13.7	110
64	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.	11.2	109
65	New Insights into Ethene Epoxidation on Two Oxidized Ag{111} Surfaces. Journal of the American Chemical Society, 2003, 125, 5620-5621.	13.7	108
66	Trends in the Chemisorption of Aromatic Molecules on a Pt(111) Surface:â€‰ Benzene, Naphthalene, and Anthracene from First Principles Calculations. Journal of Physical Chemistry B, 2004, 108, 12084-12091.	2.6	104
67	Relationship between Carbon Nitride Structure and Exciton Binding Energies: A DFT Perspective. Journal of Physical Chemistry C, 2015, 119, 25188-25196.	3.1	104
68	Influence of the Hydroxylation of Î³-Al2O3Surfaces on the Stability and Diffusion of Single Pd Atoms:Â A DFT Study. Journal of Physical Chemistry B, 2006, 110, 1759-1767.	2.6	103
69	Unravelling the Mechanism of Glycerol Hydrogenolysis over Rhodium Catalyst through Combined Experimentalâ€“Theoretical Investigations. Chemistry - A European Journal, 2011, 17, 14288-14299.	3.3	99
70	Structure and contrast in scanning tunneling microscopy of oxides: FeO monolayer on Pt(111). Physical Review B, 1996, 54, R11145-R11148.	3.2	98
71	Critical Role of the Semiconductorâ€“Electrolyte Interface in Photocatalytic Performance for Water-Splitting Reactions Using Ta₃N₅ Particles. Chemistry of Materials, 2014, 26, 4812-4825.	6.7	98
72	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.	3.1	97

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73	The adsorption of CO on Au(111) at elevated pressures studied by STM, RAIRS and DFT calculations. Surface Science, 2004, 566-568, 995-1000.	1.9	96
74	Heterogeneous Catalysis through Subsurface Sites. Journal of the American Chemical Society, 2000, 122, 1796-1801.	13.7	94
75	Chemisorption and Transformation of CHx Fragments (x = 0â^'3) on a Pd(111) Surface:â€‰ A Periodic Density Functional Study. Journal of Physical Chemistry B, 1998, 102, 1578-1585.	2.6	92
76	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.	11.3	92
77	Origin of the Enhanced Visible-Light Absorption in N-Doped Bulk Anatase TiO₂ from First-Principles Calculations. Journal of Physical Chemistry C, 2011, 115, 19394-19404.	3.1	91
78	Comparative DFT study of the adsorption of 1,3-butadiene, 1-butene and 2-cis/trans-butenes on the Pt(111) and Pd(111) surfaces. Surface Science, 2004, 549, 121-133.	1.9	90
79	Impacts of electrode potentials and solvents on the electroreduction of CO₂: a comparison of theoretical approaches. Physical Chemistry Chemical Physics, 2015, 17, 13949-13963.	2.8	90
80	Chirality forces. Journal of the American Chemical Society, 1987, 109, 2887-2894.	13.7	87
81	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.	2.8	86
82	Câ€“H versus Oâ€“H Bond Dissociation for Alcohols on a Rh(111) Surface: A Strong Assistance from Hydrogen Bonded Neighbors. ACS Catalysis, 2011, 1, 1430-1440.	11.2	85
83	Titaniaâ€Supported Catalysts for Levulinic Acid Hydrogenation: Influence of Support and its Impact on Î³â€Valerolactone Yield. ChemSusChem, 2015, 8, 1538-1547.	6.8	85
84	Nucleation ofPdn(n=1â€“5)clusters and wetting of Pd particles onÎ³â^'Al2O3surfaces: A density functional theory study. Physical Review B, 2007, 75, .	3.2	84
85	Computationally Exploring Confinement Effects in the Methane-to-Methanol Conversion Over Iron-Oxo Centers in Zeolites. ACS Catalysis, 2016, 6, 8404-8409.	11.2	83
86	Interpretation of STM images: copper-phthalocyanine on copper. Surface Science, 1992, 271, 387-394.	1.9	82
87	On the Surface Chemistry of Iron Oxides in Reactive Gas Atmospheres. Angewandte Chemie - International Edition, 2011, 50, 1584-1588.	13.8	82
88	Interplay between molecular adsorption and metalâ€“support interaction for small supported metal clusters: CO and C2H4 adsorption on Pd4/Î³Pd4/Î³-Al2O3. Journal of Catalysis, 2007, 247, 339-355.	6.2	80
89	Solvation free energies for periodic surfaces: comparison of implicit and explicit solvation models. Physical Chemistry Chemical Physics, 2016, 18, 31850-31861.	2.8	80
90	Surface Temperature Dependence of Rotational Excitation ofH2Scattered from Pd(111). Physical Review Letters, 2001, 87, 127601.	7.8	79

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91	Intermediates in the hydrogenation of benzene to cyclohexene on Pt(111) and Pd(111): A comparison from DFT calculations. Surface Science, 2006, 600, 1339-1350.	1.9	79
92	Anionic or Cationic S-Doping in Bulk Anatase TiO₂: Insights on Optical Absorption from First Principles Calculations. Journal of Physical Chemistry C, 2013, 117, 8892-8902.	3.1	78
93	Assessing a First-Principles Model of an Electrochemical Interface by Comparison with Experiment. Journal of Physical Chemistry C, 2016, 120, 5619-5623.	3.1	78
94	Atomic adsorbate identification with the STM: a theoretical approach. Surface Science, 1997, 374, 406-417.	1.9	77
95	Platinum Nanoclusters Stabilized on Î³-Alumina by Chlorine Used As a Capping Surface Ligand: A Density Functional Theory Study. ACS Catalysis, 2012, 2, 1346-1357.	11.2	77
96	A theoretical analysis of the site dependence of the shape of a molecule in STM images. Surface Science, 1994, 304, L445-L450.	1.9	76
97	Coverage Dependent Adsorption of Acrolein on Pt(111) from a Combination of First Principle Theory and HREELS Study. Journal of Physical Chemistry B, 2004, 108, 9085-9093.	2.6	75
98	Dynamics of Surface Alloys: Rearrangement of Pd/Ag(111) Induced by CO and O₂. Journal of Physical Chemistry C, 2019, 123, 8312-8323.	3.1	75
99	STM and chemistry: a qualitative molecular orbital understanding of the image of CO on a Pt surface. Surface Science, 1996, 360, 128-136.	1.9	74
100	Theoretical Study of Hydroxylated and Dehydroxylated Surfaces of a Cristobalite Model of Silica. Journal of Physical Chemistry B, 1997, 101, 8197-8203.	2.6	74
101	Adsorption of unsaturated aldehydes on the (111) surface of a Ptâ€“Fe alloy catalyst from first principles. Journal of Catalysis, 2003, 217, 354-366.	6.2	73
102	From Î³-alumina to supported platinum nanoclusters in reforming conditions: 10years of DFT modeling and beyond. Journal of Catalysis, 2013, 308, 328-340.	6.2	73
103	CH3ReO3 on Î³-Al2O3: Understanding Its Structure, Initiation, and Reactivity in Olefin Metathesis. Angewandte Chemie - International Edition, 2007, 46, 3870-3873.	13.8	72
104	Stability of intermediates in the glycerol hydrogenolysis on transition metal catalysts from first principles. Physical Chemistry Chemical Physics, 2011, 13, 1448-1456.	2.8	72
105	Key Role of Anionic Doping for H₂ Production from Formic Acid on Pd(111). ACS Catalysis, 2017, 7, 1955-1959.	11.2	72
106	Role of Hydrogen Species in Palladium-Catalyzed Alkyne Hydrogenation. Journal of Physical Chemistry C, 2010, 114, 2293-2299.	3.1	71
107	Nature and Structure of Aluminum Surface Sites Grafted on Silica from a Combination of High-Field Aluminum-27 Solid-State NMR Spectroscopy and First-Principles Calculations. Journal of the American Chemical Society, 2012, 134, 6767-6775.	13.7	71
108	Rational design of selective metal catalysts for alcohol amination with ammonia. Nature Catalysis, 2019, 2, 773-779.	34.4	70

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109	Structure of the Diamineâ^'Rh(I) Precursor in the Asymmetric Hydride Transfer Reduction of Ketones: A Theoretical and Experimental Approach. Journal of the American Chemical Society, 1998, 120, 1441-1446.	13.7	69
110	Adsorption and energetics of isolated CO molecules on Pd(111). Surface Science, 2000, 453, 25-31.	1.9	68
111	A multiscale theoretical methodology for the calculation of electrochemical observables from ab initio data: Application to the oxygen reduction reaction in a Pt(111)-based polymer electrolyte membrane fuel cell. Electrochimica Acta, 2011, 56, 10842-10856.	5.2	68
112	Acetylene structure and dynamics on Pd(111). Physical Review B, 1998, 57, R12705-R12708.	3.2	66
113	Formation of Chiral Domains for Tartaric Acid on Cu(110):Â A Combined DFT and Kinetic Monte Carlo Study. Journal of Physical Chemistry B, 2004, 108, 11035-11043.	2.6	66
114	Evaluating the Risk of Câ€“C Bond Formation during Selective Hydrogenation of Acetylene on Palladium. ACS Catalysis, 2018, 8, 1662-1671.	11.2	65
115	Transformation of molecular oxygen on a platinum surface:â€ƒA theoretical calculation of STM images. Physical Review B, 1999, 59, 15437-15445.	3.2	64
116	Surface ReO_x Sites on Al₂O₃ and Their Molecular Structureâ€“Reactivity Relationships for Olefin Metathesis. ACS Catalysis, 2015, 5, 1432-1444.	11.2	64
117	CO on Pt(111): binding site assignment from the interplay between measured and calculated STM images. Chemical Physics Letters, 1999, 299, 403-409.	2.6	62
118	A Density Functional Study of Adsorption Structures of Unsaturated Aldehydes on Pt(111): A Key Factor for Hydrogenation Selectivity. Journal of Catalysis, 2002, 211, 398-406.	6.2	62
119	Breaking the NO bond on Rh, Pd, and Pd3Mn alloy (100) surfaces: A quantum chemical comparison of reaction paths. Journal of Chemical Physics, 2001, 115, 8101-8111.	3.0	61
120	Specific Ethene Surface Activation on Silver Oxide Covered Ag{111} from the Interplay of STM Experiment and Theory. Journal of the American Chemical Society, 2003, 125, 3119-3125.	13.7	61
121	Atomic Scale Insights on Chlorinated Î³-Alumina Surfaces. Journal of the American Chemical Society, 2008, 130, 11030-11039.	13.7	61
122	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.	11.2	61
123	Selective Elimination of Alkyldibenzothiophenes from Gas Oil by Formation of Insoluble Charge-Transfer Complexes. Energy & Fuels, 1999, 13, 881-887.	5.1	60
124	Reconstruction and stability of Î²-cristobalite 001, 101, and 111 surfaces during dehydroxylation. Physical Chemistry Chemical Physics, 2010, 12, 14930.	2.8	60
125	Heterogeneous Transformation of Glycerol to Lactic Acid. Topics in Catalysis, 2012, 55, 474-479.	2.8	60
126	Multiscale Modeling of Chemistry in Water: Are We There Yet?. Journal of Chemical Theory and Computation, 2013, 9, 5567-5577.	5.3	59

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127	Ab Initio Study of the Structure of the Î±-MoO3 Solid and Study of the Adsorption of H2O and CO Molecules on Its (100) Surface. The Journal of Physical Chemistry, 1996, 100, 10681-10688.	2.9	58
128	Tetrahydrofuran in TiCl₄/THF/MgCl₂: a Non-Innocent Ligand for Supported Zieglerâ€“Natta Polymerization Catalysts. ACS Catalysis, 2013, 3, 52-56.	11.2	58
129	Electronic and Chemical Properties of the Pt80Fe20(111) Alloy Surface: A Theoretical Study of the Adsorption of Atomic H, CO, and Unsaturated Molecules. Journal of Catalysis, 1996, 164, 152-165.	6.2	56
130	.eta.2 versus .eta.1 coordination of aldehydes and ketones in organometallic complexes. A semiempirical theoretical study. Journal of the American Chemical Society, 1992, 114, 2446-2455.	13.7	55
131	Scanning-tunneling-microscopy study of the surface diffusion of sulfur on Re(0001). Physical Review B, 1993, 47, 2320-2328.	3.2	55
132	Affordable Estimation of Solvation Contributions to the Adsorption Energies of Oxygenates on Metal Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 5578-5582.	3.1	54
133	Active sites of olefin metathesis on molybdena-alumina system: A periodic DFT study. Journal of Catalysis, 2008, 256, 1-14.	6.2	53
134	Electronic properties of PbX₃CH₃NH₃ (X = Cl, Br, I) compounds for photovoltaic and photocatalytic applications. Physical Chemistry Chemical Physics, 2015, 17, 2199-2209.	2.8	52
135	Selectivity Control for the Catalytic 1,3-Butadiene Hydrogenation on Pt(111) and Pd(111) Surfaces:Â Radical versus Closed-Shell Intermediates. Journal of Physical Chemistry B, 2005, 109, 14175-14182.	2.6	51
136	Highly selective hydrogenation of butadiene on Pt/Sn alloy elucidated by first-principles calculations. Journal of Catalysis, 2010, 275, 129-139.	6.2	51
137	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.	4.1	51
138	Imaging a p(2 Ã— 2) layer of sulfur on Re(0001) with the scanning tunneling microscope: an experimental and theoretical study of the effect of adsorption site and tip structure. Surface Science, 1994, 315, 127-142.	1.9	50
139	Controlled Interactions between Anhydrous Keggin-Type Heteropolyacids and Silica Support: Preparation and Characterization of Well-Defined Silica-Supported Polyoxometalate Species. Journal of Physical Chemistry C, 2010, 114, 19024-19034.	3.1	50
140	Dilute Alloys Based on Au, Ag, or Cu for Efficient Catalysis: From Synthesis to Active Sites. Chemical Reviews, 2022, 122, 8758-8808.	47.7	50
141	Are electronic interference effects important for STM imaging of substrates and adsorbates?. Ultramicroscopy, 1992, 42-44, 115-121.	1.9	48
142	The superacidity of sulfated zirconia: an ab-initio quantum mechanical study. The Journal of Physical Chemistry, 1993, 97, 11501-11509.	2.9	48
143	Interpretation of STM images: the MoS2 surface. Surface Science, 1996, 367, 209-220.	1.9	48
144	Adsorption of Î±,Î²-Unsaturated Aldehydes on Pt(111) and Ptâ^'Sn Alloys: II. Crotonaldehyde. Journal of Physical Chemistry C, 2009, 113, 13947-13967.	3.1	48

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145	Enhanced Kinetics of Hole Transfer and Electrocatalysis during Photocatalytic Oxygen Evolution by Cocatalyst Tuning. ACS Catalysis, 2016, 6, 4117-4126.	11.2	48
146	Characterizing Slight Structural Disorder in Solids by Combined Solid-State NMR and First Principles Calculations. Journal of Physical Chemistry A, 2009, 113, 902-911.	2.5	47
147	Dehydrogenation mechanisms of methyl-cyclohexane on Î³-Al2O3 supported Pt13: Impact of cluster ductility. Journal of Catalysis, 2019, 370, 118-129.	6.2	47
148	Evolution of Metastable Structures at Bimetallic Surfaces from Microscopy and Machine-Learning Molecular Dynamics. Journal of the American Chemical Society, 2020, 142, 15907-15916.	13.7	47
149	Influence of the Surface Atom Metallic Coordination in the Adsorption of Ethylene on a Platinum Surface: A Theoretical Study. The Journal of Physical Chemistry, 1994, 98, 10906-10912.	2.9	46
150	Comparison of the nature of the hydrogen-metal bond on Pd(111) and Ni(111) by a periodic density functional method. Surface Science, 1996, 356, L403-L409.	1.9	46
151	Ab initiocalculations of scanning tunneling microscopy images within a scattering formalism. Physical Review B, 1999, 60, 1989-1999.	3.2	46
152	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.	3.1	46
153	Reaction product-driven restructuring and assisted stabilization of a highly dispersed Rh-on-ceria catalyst. Nature Catalysis, 2022, 5, 119-127.	34.4	46
154	Ab initio study of the bare and hydrated (001) surface of tetragonal zirconia. Surface Science, 1992, 275, 482-492.	1.9	45
155	H-induced reconstructions on Pd(110). Physical Review B, 1998, 57, 12482-12491.	3.2	45
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