William F Schneider

List of Publications by Year
in descending order

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214 papers	15,830 citations	22099 59 h-index	20307 116 g-index
232 all docs	232 docs citations	232 times ranked	13709 citing authors

#	Article	IF	Citations
1	CO and C3H6 poisoning of hydrogen permeation across Pd77Ag23 alloy membranes: A comparative study with pure palladium. Chemical Engineering Journal, 2022, 430, 133080.	6.6	14
2	Consequences of adsorbate-adsorbate interactions for apparent kinetics of surface catalytic reactions. Journal of Catalysis, 2022, 405, 410-418.	3.1	12
3	Observation and rationalization of nitrogen oxidation enabled only by coupled plasma and catalyst. Nature Communications, 2022, 13, 402.	5.8	23
4	Recent Advances in Plasma Catalysis. Journal of Physical Chemistry C, 2022, 126, 9611-9614.	1.5	8
5	Recent Advances in Plasma Catalysis. Industrial & Engineering Chemistry Research, 2022, 61, 7675-7678.	1.8	0
6	Effects of BrÃ¸nsted acid site proximity in chabazite zeolites on OH infrared spectra and protolytic propane cracking kinetics. Journal of Catalysis, 2021, 395, 210-226.	3.1	27
7	Inelastic Neutron Scattering Observation of Plasma-Promoted Nitrogen Reduction Intermediates on Ni/Î³-Al₂O₃. ACS Energy Letters, 2021, 6, 2048-2053.	8.8	20
8	DFT and Microkinetic Comparison of Ru-Doped Porphyrin-like Graphene and Nanotubes toward Catalytic Formic Acid Decomposition and Formation. Journal of Physical Chemistry C, 2021, 125, 18673-18683.	1.5	4
9	Plasma-catalyst modeling for materials selection: challenges and opportunities in nitrogen oxidation. Journal Physics D: Applied Physics, 2021, 54, 454004.	1.3	6
10	Adsorbate Free Energies from DFT-Derived Translational Energy Landscapes. Journal of Physical Chemistry C, 2021, 125, 20331-20342.	1.5	10
11	Plasma Catalysis for Ammonia Synthesis: A Microkinetic Modeling Study on the Contributions of Eleyâ€“Rideal Reactions. ACS Sustainable Chemistry and Engineering, 2021, 9, 13151-13163.	3.2	45
12	Comparison of Coverage-Dependent Binding Energy Models for Mean-Field Microkinetic Rate Predictions. Langmuir, 2020, 36, 465-474.	1.6	19
13	Solvation and Mobilization of Copper Active Sites in Zeolites by Ammonia: Consequences for the Catalytic Reduction of Nitrogen Oxides. Accounts of Chemical Research, 2020, 53, 1881-1892.	7.6	78
14	Plasma-Catalytic Ammonia Synthesis beyond the Equilibrium Limit. ACS Catalysis, 2020, 10, 6726-6734.	5.5	78
15	Effects of dioxygen pressure on rates of NOx selective catalytic reduction with NH3 on Cu-CHA zeolites. Journal of Catalysis, 2020, 389, 140-149.	3.1	44
16	Experimental and Computational Investigation of the Role of P in Moderating Ethane Dehydrogenation Performance over Ni-Based Catalysts. Industrial & Engineering Chemistry Research, 2020, 59, 12666-12676.	1.8	14
17	Predicted Influence of Plasma Activation on Nonoxidative Coupling of Methane on Transition Metal Catalysts. ACS Sustainable Chemistry and Engineering, 2020, 8, 6043-6054.	3.2	38
18	DFT and microkinetic comparison of Pt, Pd and Rh-catalyzed ammonia oxidation. Journal of Catalysis, 2020, 383, 322-330.	3.1	33

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19	Characteristics of Impactful Computational Contributions to The Journal of Physical Chemistry C. Journal of Physical Chemistry C, 2020, 124, 13509-13510.	1.5	3
20	Cooperative and Competitive Occlusion of Organic and Inorganic Structure-Directing Agents within Chabazite Zeolites Influences Their Aluminum Arrangement. Journal of the American Chemical Society, 2020, 142, 4807-4819.	6.6	97
21	Supercell Models of BrÃ¸nsted and Lewis Sites in Zeolites. , 2020, , 1355-1375.		2
22	The 2020 plasma catalysis roadmap. Journal Physics D: Applied Physics, 2020, 53, 443001.	1.3	362
23	The JPC Periodic Table. Journal of Physical Chemistry A, 2019, 123, 5837-5848.	1.1	2
24	The JPC Periodic Table. Journal of Physical Chemistry B, 2019, 123, 5973-5984.	1.2	1
25	The JPC Periodic Table. Journal of Physical Chemistry C, 2019, 123, 17063-17074.	1.5	1
26	The JPC Periodic Table. Journal of Physical Chemistry Letters, 2019, 10, 4051-4062.	2.1	2
27	Consequences of exchange-site heterogeneity and dynamics on the UV-visible spectrum of Cu-exchanged SSZ-13. Chemical Science, 2019, 10, 2373-2384.	3.7	80
28	Structure- and Temperature-Dependence of Pt-Catalyzed Ammonia Oxidation Rates and Selectivities. ACS Catalysis, 2019, 9, 2407-2414.	5.5	58
29	Influence of the N,N,N-Trimethyl-1-adamantyl Ammonium Structure-Directing Agent on Al Substitution in SSZ-13 Zeolite. Journal of Physical Chemistry C, 2019, 123, 17454-17458.	1.5	20
30	Water-Mediated Reduction of Aqueous N-Nitrosodimethylamine with Pd. Environmental Science & Technology, 2019, 53, 7551-7563.	4.6	11
31	Progress in Accurate Chemical Kinetic Modeling, Simulations, and Parameter Estimation for Heterogeneous Catalysis. ACS Catalysis, 2019, 9, 6624-6647.	5.5	134
32	Distinguishing Plasma Contributions to Catalyst Performance in Plasma-Assisted Ammonia Synthesis. ACS Sustainable Chemistry and Engineering, 2019, 7, 8621-8630.	3.2	98
33	The impact of transition metal catalysts on macroscopic dielectric barrier discharge (DBD) characteristics in an ammonia synthesis plasma catalysis reactor. Journal Physics D: Applied Physics, 2019, 52, 224002.	1.3	57
34	Catalysis Enabled by Plasma Activation of Strong Chemical Bonds: A Review. ACS Energy Letters, 2019, 4, 1115-1133.	8.8	212
35	Spectroscopic and kinetic responses of Cu-SSZ-13 to SO2 exposure and implications for NOx selective catalytic reduction. Applied Catalysis A: General, 2019, 574, 122-131.	2.2	48
36	Role of Molecular Modeling in the Development of CO₂â€“Reactive Ionic Liquids. Chemical Reviews, 2018, 118, 5242-5260.	23.0	68

#	Article	IF	Citations
37	Machine Learning. Journal of Physical Chemistry A, 2018, 122, 879-879.	1.1	7
38	Machine Learning. Journal of Physical Chemistry B, 2018, 122, 1347-1347.	1.2	4
39	Machine Learning. Journal of Physical Chemistry Letters, 2018, 9, 569-569.	2.1	3
40	Benchmark First-Principles Calculations of Adsorbate Free Energies. ACS Catalysis, 2018, 8, 1945-1954.	5.5	43
41	Overcoming ammonia synthesis scaling relations with plasma-enabled catalysis. Nature Catalysis, 2018, 1, 269-275.	16.1	348
42	Zeolite Adsorption Free Energies from ab Initio Potentials of Mean Force. Journal of Chemical Theory and Computation, 2018, 14, 929-938.	2.3	43
43	First-Principles Comparison of Proton and Divalent Copper Cation Exchange Energy Landscapes in SSZ-13 Zeolite. Journal of Physical Chemistry C, 2018, 122, 23564-23573.	1.5	35
44	Supercell Models of BrÃ¸nsted and Lewis Sites in Zeolites. , 2018, , 1-21.		0
45	First-Principles Analysis of Site- and Condition-Dependent Fe Speciation in SSZ-13 and Implications for Catalyst Optimization. ACS Catalysis, 2018, 8, 10119-10130.	5.5	41
46	Beyond fossil fuelâ€“driven nitrogen transformations. Science, 2018, 360, .	6.0	1,379
47	Hybrid Computational Strategy for Predicting CO₂ Solubilities in Reactive Ionic Liquids. Journal of Physical Chemistry C, 2018, 122, 14213-14221.	1.5	11
48	Ion Transport in Solvent-Free, Crosslinked, Single-Ion Conducting Polymer Electrolytes for Post-Lithium Ion Batteries. Batteries, 2018, 4, 28.	2.1	40
49	Experimental and Computational Interrogation of Fast SCR Mechanism and Active Sites on H-Form SSZ-13. ACS Catalysis, 2017, 7, 5087-5096.	5.5	53
50	Adsorption Energy Correlations at the Metalâ€“Support Boundary. ACS Catalysis, 2017, 7, 4707-4715.	5.5	49
51	Binary Approach to Ternary Cluster Expansions: NOâ€“Oâ€“Vacancy System on Pt(111). Journal of Physical Chemistry C, 2017, 121, 7344-7354.	1.5	21
52	Atomic-Scale Structural Evolution of Rh(110) during Catalysis. ACS Catalysis, 2017, 7, 664-674.	5.5	20
53	Importance of metal-oxide interfaces in heterogeneous catalysis: A combined DFT, microkinetic, and experimental study of water-gas shift on Au/MgO. Journal of Catalysis, 2017, 345, 157-169.	3.1	109
54	Participation of interfacial hydroxyl groups in the water-gas shift reaction over Au/MgO catalysts. Catalysis Science and Technology, 2017, 7, 5257-5266.	2.1	19

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55	New Physical Insights from a Computational Catalysis Perspective. Journal of Physical Chemistry C, 2017, 121, 15491-15492.	1.5	1
56	Rationalizing the light-induced phase separation of mixed halide organicâ€“inorganic perovskites. Nature Communications, 2017, 8, 200.	5.8	399
57	Dynamic multinuclear sites formed by mobilized copper ions in NO _x selective catalytic reduction. Science, 2017, 357, 898-903.	6.0	667
58	Band structure of germanium carbides for direct bandgap silicon photonics. Journal of Applied Physics, 2016, 120, .	1.1	25
59	Catalysis in a Cage: Condition-Dependent Speciation and Dynamics of Exchanged Cu Cations in SSZ-13 Zeolites. Journal of the American Chemical Society, 2016, 138, 6028-6048.	6.6	588
60	Band Anticrossing in Dilute Germanium Carbides Using Hybrid Density Functionals. Journal of Electronic Materials, 2016, 45, 2121-2126.	1.0	9
61	Catalysis Science of NOx Selective Catalytic Reduction With Ammonia Over Cu-SSZ-13 and Cu-SAPO-34. Advances in Catalysis, 2016, , 1-107.	0.1	55
62	Anion Dependent Dynamics and Water Solubility Explained by Hydrogen Bonding Interactions in Mixtures of Water and Aprotic Heterocyclic Anion Ionic Liquids. Journal of Physical Chemistry B, 2016, 120, 12679-12686.	1.2	18
63	Periodic DFT Characterization of NO_x Adsorption in Cu-Exchanged SSZ-13 Zeolite Catalysts. Journal of Physical Chemistry C, 2016, 120, 27934-27943.	1.5	29
64	Tracking Iodide and Bromide Ion Segregation in Mixed Halide Lead Perovskites during Photoirradiation. ACS Energy Letters, 2016, 1, 290-296.	8.8	321
65	CO₂ Chemistry of Phenolate-Based Ionic Liquids. Journal of Physical Chemistry B, 2016, 120, 1509-1517.	1.2	67
66	Band structure and characterization of dilute Ge:C alloys. , 2015, , .		0
67	First-Principles Analysis of Structure Sensitivity in NO Oxidation on Pt. ACS Catalysis, 2015, 5, 1087-1099.	5.5	35
68	Comparison of cluster expansion fitting algorithms for interactions at surfaces. Surface Science, 2015, 640, 104-111.	0.8	38
69	Speciation, Conductivities, Diffusivities, and Electrochemical Reduction as a Function of Water Content in Mixtures of Hydrated Chromium Chloride/Choline Chloride. Journal of Physical Chemistry B, 2015, 119, 6018-6023.	1.2	32
70	Differences Between Thermal and Laser-Induced Diffusion. Physical Review Letters, 2015, 114, 146104.	2.9	15
71	DFT Analysis of NO Oxidation Intermediates on Undoped and Doped LaCoO₃ Perovskite. Journal of Physical Chemistry C, 2015, 119, 20488-20494.	1.5	39
72	Performance implications of chemical absorption for the carbon-dioxide-cofluid refrigeration cycle. International Journal of Refrigeration, 2014, 46, 196-206.	1.8	12

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73	Implications of coverage-dependent O adsorption for catalytic NO oxidation on the late transition metals. Catalysis Science and Technology, 2014, 4, 4356-4365.	2.1	59
74	Isolation of the Copper Redox Steps in the Standard Selective Catalytic Reduction on Cuâ€SSZâ€13. Angewandte Chemie - International Edition, 2014, 53, 11828-11833.	7.2	305
75	Identification of the active Cu site in standard selective catalytic reduction with ammonia on Cu-SSZ-13. Journal of Catalysis, 2014, 312, 87-97.	3.1	286
76	NO oxidation: A probe reaction on Cu-SSZ-13. Journal of Catalysis, 2014, 312, 179-190.	3.1	155
77	First-principles reaction site model for coverage-sensitive surface reactions: Pt(111)â€“O temperature programmed desorption. Surface Science, 2014, 622, L1-L6.	0.8	24
78	Coverage-Dependent Adsorption at a Low Symmetry Surface: DFT and Statistical Analysis of Oxygen Chemistry on Kinked Pt(321). Topics in Catalysis, 2014, 57, 89-105.	1.3	24
79	DFT comparison of intrinsic WGS kinetics over Pd and Pt. Journal of Catalysis, 2014, 320, 106-117.	3.1	106
80	Trends in Atomic Adsorption on Pt₃M(111) Transition Metal Bimetallic Surface Overlayers. Journal of Physical Chemistry C, 2014, 118, 8342-8349.	1.5	16
81	Competing Reactions of CO₂ with Cations and Anions in Azolide Ionic Liquids. ChemSusChem, 2014, 7, 1970-1975.	3.6	59
82	Chemically Tunable Ionic Liquids with Aprotic Heterocyclic Anion (AHA) for CO₂ Capture. Journal of Physical Chemistry B, 2014, 118, 5740-5751.	1.2	211
83	LDA+U evaluation of the stability of low-index facets of LaCoO3 perovskite. Surface Science, 2014, 619, 71-76.	0.8	23
84	Solidâ€State Covalent Capture of CO₂ by Using Nâ€Heterocyclic Carbenes. Chemistry - A European Journal, 2013, 19, 11134-11138.	1.7	30
85	Structure and Dynamics of Uranyl(VI) and Plutonyl(VI) Cations in Ionic Liquid/Water Mixtures via Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2013, 117, 10852-10868.	1.2	35
86	Structure Sensitivity Study of Waterborne Contaminant Hydrogenation Using Shape- and Size-Controlled Pd Nanoparticles. ACS Catalysis, 2013, 3, 453-463.	5.5	74
87	Development and application of effective pairwise potentials for UO2n+, NpO2n+, PuO2n+, and AmO2n+ (n = 1, 2) ions with water. Physical Chemistry Chemical Physics, 2013, 15, 15954.	1.3	42
88	Experimental and Computational Investigation of Effect of Sr on NO Oxidation and Oxygen Exchange for La_{1â€“x}Sr_xCoO₃ Perovskite Catalysts. ACS Catalysis, 2013, 3, 2719-2728.	5.5	74
89	Site specific carboxylation of abnormal anionic N-heterocyclic dicarbenes with CO2. Chemical Communications, 2013, 49, 11527.	2.2	23
90	First-principles Thermodynamic Models in Heterogeneous Catalysis. RSC Catalysis Series, 2013, , 59-115.	0.1	9

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91	Evaluation of ionic fluids as lubricants in manufacturing. Journal of Manufacturing Processes, 2013, 15, 414-418.	2.8	23
92	Catalytic Hydrogenation of CO₂ to Formic Acid with Silicaâ€Tethered Iridium Catalysts. ChemCatChem, 2013, 5, 1769-1771.	1.8	100
93	First-principles-guided design of ionic liquids for CO2 capture. Physical Chemistry Chemical Physics, 2012, 14, 13163.	1.3	77
94	Performance of Cluster Expansions of Coverage-Dependent Adsorption of Atomic Oxygen on Pt(111). Journal of Chemical Theory and Computation, 2012, 8, 264-273.	2.3	87
95	Comparative chemistries of CO and NO oxidation over RuO₂(110): insights from first-principles thermodynamics and kinetics. Molecular Simulation, 2012, 38, 615-630.	0.9	12
96	Interplay between Subsurface Ordering, Surface Segregation, and Adsorption on Ptâ€“Ti(111) Near-Surface Alloys. Langmuir, 2012, 28, 4683-4693.	1.6	29
97	Influence of Dipoleâ€“Dipole Interactions on Coverage-Dependent Adsorption: CO and NO on Pt(111). Langmuir, 2012, 28, 8408-8417.	1.6	67
98	Configurational control in catalysis: Perspective on Hess et al., One-dimensional confinement in heterogeneous catalysis: Trapped oxygen on RuO2(110) model catalysts. Surface Science, 2012, 606, 1351-1352.	0.8	6
99	How low can you go? Minimum energy pathways for O2 dissociation on Pt(111). Physical Chemistry Chemical Physics, 2012, 14, 16677.	1.3	50
100	Critical Review of Pd-Based Catalytic Treatment of Priority Contaminants in Water. Environmental Science & Technology, 2012, 46, 3655-3670.	4.6	373
101	Response to Comment on â€œCritical Review of Pd-Based Catalytic Treatment of Priority Contaminants in Waterâ€• Environmental Science & Technology, 2012, 46, 11469-11470.	4.6	10
102	Aqueous N2O Reduction with H2 Over Pd-Based Catalyst: Mechanistic Insights From Experiment and Simulation. Topics in Catalysis, 2012, 55, 300-312.	1.3	11
103	Integrated operando X-ray absorption and DFT characterization of Cuâ€“SSZ-13 exchange sites during the selective catalytic reduction of NO with NH3. Catalysis Today, 2012, 184, 129-144.	2.2	212
104	Accurate coverage-dependence incorporated into first-principles kinetic models: Catalytic NO oxidation on Pt (111). Journal of Catalysis, 2012, 286, 88-94.	3.1	146
105	Ordering and Oxygen Adsorption in Auâ€“Pt/Pt(111) Surface Alloys. Journal of Physical Chemistry C, 2011, 115, 17915-17924.	1.5	40
106	Potential Energy Surfaces for Oxygen Adsorption, Dissociation, and Diffusion at the Pt(321) Surface. Langmuir, 2011, 27, 8177-8186.	1.6	34
107	Direct Control of Electron Transfer to the Surface-CO Bond on a Pt/TiO₂Catalytic Diode. Journal of the American Chemical Society, 2011, 133, 16459-16467.	6.6	35
108	First-principles cluster expansion study of missing-row reconstructions of fcc (110) surfaces. Physical Review B, 2011, 83, .	1.1	24

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109	DFT Comparison of Nâ€Nitrosodimethylamine Decomposition Pathways Over Ni and Pd. ChemCatChem, 2011, 3, 898-903.	1.8	11
110	Adsorption and reactions of NOx on RuO2(110). Catalysis Today, 2011, 165, 49-55.	2.2	22
111	DFTâ€Based Coverageâ€Dependent Model of Ptâ€Catalyzed NO Oxidation. ChemCatChem, 2010, 2, 1450-1460.	1.8	91
112	Computational Comparison of Tethering Strategies for Amine Functionalised Ionic Liquids. ACS Symposium Series, 2010, , 419-430.	0.5	10
113	Equimolar CO₂ Absorption by Anion-Functionalized Ionic Liquids. Journal of the American Chemical Society, 2010, 132, 2116-2117.	6.6	791
114	Computational Comparison of the Reactions of Substituted Amines with CO₂. ChemSusChem, 2010, 3, 931-938.	3.6	51
115	Influence of Î±-alumina supports on oxygen binding to Pd, Ag, Pt, and Au. Chemical Physics Letters, 2010, 484, 231-236.	1.2	17
116	Molecular Design of High Capacity, Low Viscosity, Chemically Tunable Ionic Liquids for CO₂ Capture. Journal of Physical Chemistry Letters, 2010, 1, 3494-3499.	2.1	378
117	Bulk and Surface Properties of Rutile TiO₂ from Self-Consistent-Charge Density Functional Tight Binding. Journal of Chemical Theory and Computation, 2010, 6, 499-507.	2.3	34
118	Enhancement of Oxyanion and Diatrizoate Reduction Kinetics Using Selected Azo Dyes on Pd-Based Catalysts. Environmental Science & Technology, 2010, 44, 1773-1779.	4.6	33
119	Nature and role of surface carbonates and bicarbonates in CO oxidation over RuO2. Physical Chemistry Chemical Physics, 2010, 12, 6367.	1.3	24
120	Molecular origins of surface poisoning during CO oxidation over RuO2(110). Surface Science, 2009, 603, L91-L94.	0.8	13
121	Oxygen-Coverage Effects on Molecular Dissociations at a Pt Metal Surface. Physical Review Letters, 2009, 102, 076101.	2.9	100
122	Intermediates and Spectators in O₂Dissociation at the RuO₂(110) Surface. Journal of Physical Chemistry C, 2009, 113, 15266-15273.	1.5	54
123	Density Functional Theory Comparison of Water Dissociation Steps on Cu, Au, Ni, Pd, and Pt. Journal of Physical Chemistry C, 2009, 113, 7269-7276.	1.5	257
124	DFT Investigation of Intermediate Steps in the Hydrolysis of Î±-Al₂O₃(0001). Journal of Physical Chemistry C, 2009, 113, 2149-2158.	1.5	81
125	A Periodic Density Functional Theory Analysis of CO Chemisorption on Pt(111) in the Presence of Uniform Electric Fields. Journal of Physical Chemistry A, 2009, 113, 4125-4133.	1.1	51
126	DFT characterization of coverage dependent molecular water adsorption modes on Î±-Al2O3(0001). Surface Science, 2008, 602, 268-275.	0.8	73

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127	Surface termination effects on metal atom adsorption on Î±-alumina. Surface Science, 2008, 602, 3445-3453.	0.8	31
128	Coupled theoretical and experimental analysis of surface coverage effects in Pt-catalyzed NO and O2 reaction to NO2 on Pt(111). Catalysis Today, 2008, 136, 84-92.	2.2	79
129	Thermodynamics of Environment-Dependent Oxygen Chemisorption on Pt(111). Journal of Physical Chemistry C, 2008, 112, 9559-9572.	1.5	173
130	Experimental and Computational Investigation of Gas-Phase Reaction of Chlorine with n-Propanol:â€‰ Observation of Chloropropanol Conformational Isomerization at Room Temperature. Journal of Physical Chemistry A, 2008, 112, 2773-2781.	1.1	8
131	A first-principles investigation of the effect of Pt cluster size on CO and NO oxidation intermediates and energetics. Physical Chemistry Chemical Physics, 2008, 10, 6009.	1.3	45
132	Effects of coverage on the structures, energetics, and electronics of oxygen adsorption on RuO2(110). Journal of Chemical Physics, 2007, 127, 064706.	1.2	42
133	Kinetics and mechanism of the gas phase reaction of chlorine atoms with i-propanol. Physical Chemistry Chemical Physics, 2007, 9, 4211.	1.3	15
134	Viewpoint: Chemistry for a Sustainable Future. Environmental Science & Technology, 2007, 41, 4840-4846.	4.6	32
135	Transferable Force Field for Water Adsorption in Cation-Exchanged Titanosilicates. Industrial & Engineering Chemistry Research, 2007, 46, 5754-5765.	1.8	3
136	DFT-Based Characterization of the Multiple Adsorption Modes of Nitrogen Oxides on Pt(111). Journal of Physical Chemistry C, 2007, 111, 389-397.	1.5	84
137	Catalysis by Design - Theoretical and Experimental Studies of Model Catalysts. , 2007, , .		2
138	Effect of Particle Size on the Oxidizability of Platinum Clusters. Journal of Physical Chemistry A, 2006, 110, 5839-5846.	1.1	75
139	Thermodynamic Equilibrium Compositions, Structures, and Reaction Energies of PtxOy(x= 1â^'3) Clusters Predicted from First Principles. Journal of Physical Chemistry B, 2006, 110, 16591-16599.	1.2	51
140	Theoretical Aspects of Oxide Particle Stability and Chemical Reactivity. , 2006, , 289-309.		0
141	NO oxidation over supported Pt: Impact of precursor, support, loading, and processing conditions evaluated via high throughput experimentation. Applied Catalysis B: Environmental, 2006, 67, 246-256.	10.8	86
142	Thermal decomposition of dispersed and bulk-like NOx species in model NOx trap materials. Applied Catalysis B: Environmental, 2005, 61, 164-175.	10.8	42
143	NO oxidation properties of Pt(111) revealed byab initiokinetic simulations. Physical Review B, 2005, 71, .	1.1	65
144	A thermogravimetric determination of dispersed and bulk-like barium species supported on Î³-alumina. Journal of Materials Chemistry, 2005, 15, 366-368.	6.7	11

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145	Molecular Origins of Selectivity in the Reduction of NOxby NH3. Journal of Physical Chemistry A, 2004, 108, 9365-9374.	1.1	25
146	Qualitative Differences in the Adsorption Chemistry of Acidic (CO2, SOx) and Amphiphilic (NOx) Species on the Alkaline Earth Oxides. Journal of Physical Chemistry B, 2004, 108, 273-282.	1.2	147
147	Chemistry of Sulfur Oxides on Transition Metals. III. Oxidation of SO2and Self-Diffusion of O, SO2, and SO3on Pt(111). Journal of Physical Chemistry B, 2004, 108, 13329-13340.	1.2	40
148	Chemistry of Sulfur Oxides on Transition Metals. II. Thermodynamics of Sulfur Oxides on Platinum(111). Journal of Physical Chemistry B, 2004, 108, 250-264.	1.2	43
149	CF3CH(ONO)CF3: Synthesis, IR spectrum, and use as OH radical source for kinetic and mechanistic studies. International Journal of Chemical Kinetics, 2003, 35, 159-165.	1.0	7
150	Characterization of adsorption trends of NO2, nitrite, and nitrate on MgO terraces. Surface Science, 2003, 546, 75-86.	0.8	20
151	First-Principles Characterization of NOxAdsorption on MgO. Journal of Physical Chemistry B, 2003, 107, 157-163.	1.2	44
152	Kinetics of Elementary Reactions in the Chain Chlorination of Cyclopropane. Journal of Physical Chemistry A, 2003, 107, 2003-2010.	1.1	13
153	Dramatic Cooperative Effects in Adsorption of NOx on MgO(001). Journal of Physical Chemistry B, 2002, 106, 7405-7413.	1.2	86
154	Formation of Methane Sulfinic Acid in the Gas-Phase OH-Radical Initiated Oxidation of Dimethyl Sulfoxide. Environmental Science & Technology, 2002, 36, 5155-5163.	4.6	53
155	Chemistry of Sulfur Oxides on Transition Metals I:Â Configurations, Energetics, Orbital Analyses, and Surface Coverage Effects of SO2on Pt(111). Journal of Physical Chemistry B, 2002, 106, 12575-12583.	1.2	60
156	Analysis of the thermodynamic feasibility of NOx decomposition catalysis to meet next generation vehicle NOx emissions standards. Applied Catalysis B: Environmental, 2002, 37, 263-277.	10.8	27
157	Simulated performance and cofluid dependence of a CO2-cofluid refrigeration cycle with wet compression. International Journal of Refrigeration, 2002, 25, 1123-1136.	1.8	12
158	Effect of Particle Size on the Adsorption of O and S Atoms on Pt:Â A Density-Functional Theory Study. Journal of Physical Chemistry B, 2001, 105, 7739-7747.	1.2	65
159	Combined Computational and Experimental Investigation of SOx Adsorption on MgO. Journal of Physical Chemistry B, 2001, 105, 6972-6979.	1.2	75
160	Title is missing!. Catalysis Letters, 2001, 74, 193-199.	1.4	30
161	Stability and infrared spectra of mono-, di-, and trichloromethanol. Chemical Physics Letters, 2000, 322, 97-102.	1.2	46
162	Statistical analysis of Al distributions and metal ion pairing probabilities in zeolites. Catalysis Letters, 2000, 68, 85-93.	1.4	46

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163	First-Principles Molecular Dynamics Simulations of H2O on Î±-Al2O3(0001). Journal of Physical Chemistry B, 2000, 104, 5527-5540.	1.2	213
164	CO oxidation catalyzed by Cuâ€exchanged zeolites: a density functional theory study. Catalysis Letters, 1999, 61, 179-186.	1.4	7
165	Density functional studies of adsorbates in Cu-exchanged zeolites: model comparisons and SOx binding. Physical Chemistry Chemical Physics, 1999, 1, 639-648.	1.3	41
166	Cluster Model Studies of Oxygen-Bridged Cu Pairs in Cuâ^'ZSM-5 Catalysts. Journal of Physical Chemistry B, 1999, 103, 10452-10460.	1.2	66
167	Comparison of Explicit and United Atom Models for Alkane Chains Physisorbed on Î±-Al2O3 (0001). Journal of Physical Chemistry B, 1999, 103, 3885-3895.	1.2	51
168	Theoretical analysis of oxygen-bridged Cu pairs in Cu-exchanged zeolites. Catalysis Letters, 1998, 56, 183-188.	1.4	67
169	CF₃CFHO^{â€¢} radical: Decomposition vs. reaction with O₂. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1998, 102, 1850-1856.	0.9	18
170	Atmospheric chemistry of acetone: Kinetic study of the CH3C(O)CH2O2+NO/NO2 reactions and decomposition of CH3C(O)CH2O2NO2. International Journal of Chemical Kinetics, 1998, 30, 475-489.	1.0	32
171	The Chemistry of Water on Alumina Surfaces: Reaction Dynamics from First Principles. , 1998, 282, 265-268.		512
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