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	Beyond fossil fuelâ€“driven nitrogen transformations. Science, 2018, 360, .	6.0	1,379
2	Equimolar CO₂ Absorption by Anion-Functionalized Ionic Liquids. Journal of the American Chemical Society, 2010, 132, 2116-2117.	6.6	791
3	Dynamic multinuclear sites formed by mobilized copper ions in NO _x selective catalytic reduction. Science, 2017, 357, 898-903.	6.0	667
4	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
5	The Chemistry of Water on Alumina Surfaces: Reaction Dynamics from First Principles. , 1998, 282, 265-268.		512
6	Rationalizing the light-induced phase separation of mixed halide organicâ€“inorganic perovskites. Nature Communications, 2017, 8, 200.	5.8	399
7	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
8	Critical Review of Pd-Based Catalytic Treatment of Priority Contaminants in Water. Environmental Science & Technology, 2012, 46, 3655-3670.	4.6	373
9	The 2020 plasma catalysis roadmap. Journal Physics D: Applied Physics, 2020, 53, 443001.	1.3	362
10	Overcoming ammonia synthesis scaling relations with plasma-enabled catalysis. Nature Catalysis, 2018, 1, 269-275.	16.1	348
11	Tracking Iodide and Bromide Ion Segregation in Mixed Halide Lead Perovskites during Photoirradiation. ACS Energy Letters, 2016, 1, 290-296.	8.8	321
12	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
13	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
14	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
15	First-Principles Molecular Dynamics Simulations of H2O on Î±-Al2O3(0001). Journal of Physical Chemistry B, 2000, 104, 5527-5540.	1.2	213
16	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
17	Catalysis Enabled by Plasma Activation of Strong Chemical Bonds: A Review. ACS Energy Letters, 2019, 4, 1115-1133.	8.8	212
18	Chemically Tunable Ionic Liquids with Aprotic Heterocyclic Anion (AHA) for CO₂ Capture. Journal of Physical Chemistry B, 2014, 118, 5740-5751.	1.2	211

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19	Thermodynamics of Environment-Dependent Oxygen Chemisorption on Pt(111). Journal of Physical Chemistry C, 2008, 112, 9559-9572.	1.5	173
20	The Stratospheric Fate of CF3OH. Environmental Science & Technology, 1994, 28, 1198-1200.	4.6	168
21	NO oxidation: A probe reaction on Cu-SSZ-13. Journal of Catalysis, 2014, 312, 179-190.	3.1	155
22	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
23	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
24	Progress in Accurate Chemical Kinetic Modeling, Simulations, and Parameter Estimation for Heterogeneous Catalysis. ACS Catalysis, 2019, 9, 6624-6647.	5.5	134
25	Atmospheric Chemistry of HFE-7100 (C4F9OCH3):Â Reaction with OH Radicals, UV Spectra and Kinetic Data for C4F9OCH2Â· and C4F9OCH2O2Â· Radicals, and the Atmospheric Fate of C4F9OCH2OÂ· Radicals. Journal of Physical Chemistry A, 1997, 101, 8264-8274.	1.1	120
26	Atmospheric Chemistry of the Phenoxy Radical, C6H5O(â€¢):â€‰ UV Spectrum and Kinetics of Its Reaction with NO, NO2, and O2. Journal of Physical Chemistry A, 1998, 102, 7964-7974.	1.1	110
27	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
28	DFT comparison of intrinsic WGS kinetics over Pd and Pt. Journal of Catalysis, 2014, 320, 106-117.	3.1	106
29	Cluster Models of Cu Binding and CO and NO Adsorption in Cu-Exchanged Zeolites. The Journal of Physical Chemistry, 1996, 100, 6032-6046.	2.9	100
30	Oxygen-Coverage Effects on Molecular Dissociations at a Pt Metal Surface. Physical Review Letters, 2009, 102, 076101.	2.9	100
31	Catalytic Hydrogenation of CO₂ to Formic Acid with Silicaâ€Tethered Iridium Catalysts. ChemCatChem, 2013, 5, 1769-1771.	1.8	100
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	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
34	DFTâ€Based Coverageâ€Dependent Model of Ptâ€Catalyzed NO Oxidation. ChemCatChem, 2010, 2, 1450-1460.	1.8	91
35	Density Functional Theory Study of Transformations of Nitrogen Oxides Catalyzed by Cu-Exchanged Zeolites. Journal of Physical Chemistry B, 1998, 102, 3692-3705.	1.2	90
36	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

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37	Dramatic Cooperative Effects in Adsorption of NOx on MgO(001). Journal of Physical Chemistry B, 2002, 106, 7405-7413.	1.2	86
38	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
39	The environmental impact of CFC replacements - HFCs and HCFCs. Environmental Science & Technology, 1994, 28, 320A-326A.	4.6	85
40	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
41	Kinetics and Mechanisms of the Self-Reactions of CCl3O2and CHCl2O2Radicals and Their Reactions with HO2. The Journal of Physical Chemistry, 1996, 100, 14356-14371.	2.9	81
42	DFT Investigation of Intermediate Steps in the Hydrolysis of Î±-Al₂O₃(0001). Journal of Physical Chemistry C, 2009, 113, 2149-2158.	1.5	81
43	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
44	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
45	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
46	Plasma-Catalytic Ammonia Synthesis beyond the Equilibrium Limit. ACS Catalysis, 2020, 10, 6726-6734.	5.5	78
47	First-principles-guided design of ionic liquids for CO2 capture. Physical Chemistry Chemical Physics, 2012, 14, 13163.	1.3	77
48	Combined Computational and Experimental Investigation of SOx Adsorption on MgO. Journal of Physical Chemistry B, 2001, 105, 6972-6979.	1.2	75
49	Effect of Particle Size on the Oxidizability of Platinum Clusters. Journal of Physical Chemistry A, 2006, 110, 5839-5846.	1.1	75
50	Structure Sensitivity Study of Waterborne Contaminant Hydrogenation Using Shape- and Size-Controlled Pd Nanoparticles. ACS Catalysis, 2013, 3, 453-463.	5.5	74
51	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
52	DFT characterization of coverage dependent molecular water adsorption modes on Î±-Al2O3(0001). Surface Science, 2008, 602, 268-275.	0.8	73
53	Role of Molecular Modeling in the Development of CO₂â€“Reactive Ionic Liquids. Chemical Reviews, 2018, 118, 5242-5260.	23.0	68
54	Theoretical analysis of oxygen-bridged Cu pairs in Cu-exchanged zeolites. Catalysis Letters, 1998, 56, 183-188.	1.4	67

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55	Influence of Dipoleâ€“Dipole Interactions on Coverage-Dependent Adsorption: CO and NO on Pt(111). Langmuir, 2012, 28, 8408-8417.	1.6	67
56	CO₂ Chemistry of Phenolate-Based Ionic Liquids. Journal of Physical Chemistry B, 2016, 120, 1509-1517.	1.2	67
57	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
58	First-Principles Analysis of Elementary Steps in the Catalytic Decomposition of NO by Cu-Exchanged Zeolites. Journal of Physical Chemistry B, 1997, 101, 4353-4357.	1.2	65
59	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
60	NO oxidation properties of Pt(111) revealed byab initiokinetic simulations. Physical Review B, 2005, 71, .	1.1	65
61	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
62	Bond Strength Trends in Halogenated Methanols: Evidence for Negative Hyperconjugation?. Journal of the American Chemical Society, 1995, 117, 478-485.	6.6	59
63	Hydrofluorocarbons and stratospheric ozone. Faraday Discussions, 1995, 100, 55.	1.6	59
64	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
65	Competing Reactions of CO₂ with Cations and Anions in Azolide Ionic Liquids. ChemSusChem, 2014, 7, 1970-1975.	3.6	59
66	Ab initio investigation of the heats of formation of several trifluoromethyl compounds. The Journal of Physical Chemistry, 1993, 97, 12783-12788.	2.9	58
67	Structure- and Temperature-Dependence of Pt-Catalyzed Ammonia Oxidation Rates and Selectivities. ACS Catalysis, 2019, 9, 2407-2414.	5.5	58
68	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
69	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
70	Intermediates and Spectators in O₂Dissociation at the RuO₂(110) Surface. Journal of Physical Chemistry C, 2009, 113, 15266-15273.	1.5	54
71	Cuâ^'Dinitrosyl Species in Zeolites:Â A Density Functional Molecular Cluster Study. Journal of Physical Chemistry B, 1997, 101, 6903-6913.	1.2	53
72	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

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73	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
74	The Environmental Impact of CFC Replacements HFCs and HCFCs. Environmental Science & Technology, 1994, 28, 320A-326A.	4.6	52
75	Reliability of Small Cluster Models for Cu-Exchanged Zeolites. The Journal of Physical Chemistry, 1996, 100, 9292-9301.	2.9	52
76	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
77	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
78	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
79	Computational Comparison of the Reactions of Substituted Amines with CO₂. ChemSusChem, 2010, 3, 931-938.	3.6	51
80	How low can you go? Minimum energy pathways for O2 dissociation on Pt(111). Physical Chemistry Chemical Physics, 2012, 14, 16677.	1.3	50
81	Adsorption Energy Correlations at the Metalâ€“Support Boundary. ACS Catalysis, 2017, 7, 4707-4715.	5.5	49
82	Atmospheric chemistry of trifluoromethoxy radicals: reaction with water. The Journal of Physical Chemistry, 1993, 97, 7606-7611.	2.9	48
83	Atmospheric chemistry of CH3Cl: mechanistic study of the reaction of CH2ClO2 radicals with HO2. Chemical Physics Letters, 1996, 251, 164-173.	1.2	48
84	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
85	Mechanistic study of the gas-phase reaction of CH2FO2 radicals with HO2. Chemical Physics Letters, 1994, 218, 34-42.	1.2	46
86	Stability and infrared spectra of mono-, di-, and trichloromethanol. Chemical Physics Letters, 2000, 322, 97-102.	1.2	46
87	Statistical analysis of Al distributions and metal ion pairing probabilities in zeolites. Catalysis Letters, 2000, 68, 85-93.	1.4	46
88	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
89	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
90	Rate coefficient for the reaction of hydroxymethyl radicals with chlorine and infrared spectra of chloromethanol and dichloromethanol. The Journal of Physical Chemistry, 1993, 97, 1576-1582.	2.9	44

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91	Energetics and Mechanism of Decomposition of CF3OH. The Journal of Physical Chemistry, 1996, 100, 6097-6103.	2.9	44
92	First-Principles Characterization of NOxAdsorption on MgO. Journal of Physical Chemistry B, 2003, 107, 157-163.	1.2	44
93	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
94	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
95	Benchmark First-Principles Calculations of Adsorbate Free Energies. ACS Catalysis, 2018, 8, 1945-1954.	5.5	43
96	Zeolite Adsorption Free Energies from ab Initio Potentials of Mean Force. Journal of Chemical Theory and Computation, 2018, 14, 929-938.	2.3	43
97	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
98	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
99	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
100	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
101	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
102	Theoretical Study of CO and NO Vibrational Frequencies in Cuâ”Water Clusters and Implications for Cu-Exchanged Zeolites. Journal of Physical Chemistry B, 1997, 101, 1940-1949.	1.2	40
103	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
104	Ordering and Oxygen Adsorption in Auâ€“Pt/Pt(111) Surface Alloys. Journal of Physical Chemistry C, 2011, 115, 17915-17924.	1.5	40
105	Ion Transport in Solvent-Free, Crosslinked, Single-Ion Conducting Polymer Electrolytes for Post-Lithium Ion Batteries. Batteries, 2018, 4, 28.	2.1	40
106	Simulations of hydrocarbon adsorption and subsequent water penetration on an aluminum oxide surface. Journal of Chemical Physics, 1997, 106, 7331-7342.	1.2	39
107	DFT Analysis of NO Oxidation Intermediates on Undoped and Doped LaCoO₃ Perovskite. Journal of Physical Chemistry C, 2015, 119, 20488-20494.	1.5	39
108	Comparison of cluster expansion fitting algorithms for interactions at surfaces. Surface Science, 2015, 640, 104-111.	0.8	38

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109	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
110	Thermochemistry of COF2 and Related Compounds. The Journal of Physical Chemistry, 1994, 98, 7448-7451.	2.9	35
111	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
112	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
113	First-Principles Analysis of Structure Sensitivity in NO Oxidation on Pt. ACS Catalysis, 2015, 5, 1087-1099.	5.5	35
114	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
115	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
116	Potential Energy Surfaces for Oxygen Adsorption, Dissociation, and Diffusion at the Pt(321) Surface. Langmuir, 2011, 27, 8177-8186.	1.6	34
117	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
118	DFT and microkinetic comparison of Pt, Pd and Rh-catalyzed ammonia oxidation. Journal of Catalysis, 2020, 383, 322-330.	3.1	33
119	Kinetic study of the reaction CF3O+O3â†'CF3O2+O2. Chemical Physics Letters, 1993, 213, 442-448.	1.2	32
120	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
121	Viewpoint: Chemistry for a Sustainable Future. Environmental Science & Technology, 2007, 41, 4840-4846.	4.6	32
122	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
123	Structure and bonding trends in two- and three-coordinate boron cations. Inorganic Chemistry, 1991, 30, 3919-3927.	1.9	31
124	Surface termination effects on metal atom adsorption on Î±-alumina. Surface Science, 2008, 602, 3445-3453.	0.8	31
125	Title is missing!. Catalysis Letters, 2001, 74, 193-199.	1.4	30
126	Solidâ€State Covalent Capture of CO₂ by Using Nâ€Heterocyclic Carbenes. Chemistry - A European Journal, 2013, 19, 11134-11138.	1.7	30

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127	Density functional theory description of excited-state intramolecular proton transfer. Chemical Physics Letters, 1996, 263, 414-422.	1.2	29
128	Novel Structural Modifications Associated with the Highly Efficient Internal Conversion of 2-(2â€˜-Hydroxyphenyl)benzotriazole Ultraviolet Stabilizers. Journal of the American Chemical Society, 1997, 119, 5445-5446.	6.6	29
129	Interplay between Subsurface Ordering, Surface Segregation, and Adsorption on Ptâ€“Ti(111) Near-Surface Alloys. Langmuir, 2012, 28, 4683-4693.	1.6	29
130	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
131	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
132	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
133	Molecular Origins of Selectivity in the Reduction of NOxby NH3. Journal of Physical Chemistry A, 2004, 108, 9365-9374.	1.1	25
134	Band structure of germanium carbides for direct bandgap silicon photonics. Journal of Applied Physics, 2016, 120, .	1.1	25
135	Nature and role of surface carbonates and bicarbonates in CO oxidation over RuO2. Physical Chemistry Chemical Physics, 2010, 12, 6367.	1.3	24
136	First-principles cluster expansion study of missing-row reconstructions of fcc (110) surfaces. Physical Review B, 2011, 83, .	1.1	24
137	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
138	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
139	Atmospheric Chemistry of CF3OH: Is Photolysis Important?. Environmental Science & Technology, 1995, 29, 247-250.	4.6	23
140	Kinetics and mechanism of the reaction of Cl atoms with CH2 CO (Ketene). International Journal of Chemical Kinetics, 1996, 28, 627-635.	1.0	23
141	Site specific carboxylation of abnormal anionic N-heterocyclic dicarbenes with CO2. Chemical Communications, 2013, 49, 11527.	2.2	23
142	Evaluation of ionic fluids as lubricants in manufacturing. Journal of Manufacturing Processes, 2013, 15, 414-418.	2.8	23
143	LDA+U evaluation of the stability of low-index facets of LaCoO3 perovskite. Surface Science, 2014, 619, 71-76.	0.8	23
144	Observation and rationalization of nitrogen oxidation enabled only by coupled plasma and catalyst. Nature Communications, 2022, 13, 402.	5.8	23

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145	The vibrational spectrum of FC(O)O radical: A challenging case for singleâ€reference electron correlation methods. Journal of Chemical Physics, 1995, 103, 6601-6607.	1.2	22
146	Adsorption and reactions of NOx on RuO2(110). Catalysis Today, 2011, 165, 49-55.	2.2	22
147	Atmospheric Chemistry of FNO and FNO2: Reactions of FNO with O3, O(3P), HO2, and HCl and the Reaction of FNO2 with O3. The Journal of Physical Chemistry, 1995, 99, 984-989.	2.9	21
148	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
149	Characterization of adsorption trends of NO2, nitrite, and nitrate on MgO terraces. Surface Science, 2003, 546, 75-86.	0.8	20
150	Atomic-Scale Structural Evolution of Rh(110) during Catalysis. ACS Catalysis, 2017, 7, 664-674.	5.5	20
151	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
152	Inelastic Neutron Scattering Observation of Plasma-Promoted Nitrogen Reduction Intermediates on Ni/Î³-Al₂O₃. ACS Energy Letters, 2021, 6, 2048-2053.	8.8	20
153	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
154	Comparison of Coverage-Dependent Binding Energy Models for Mean-Field Microkinetic Rate Predictions. Langmuir, 2020, 36, 465-474.	1.6	19
155	Alcoholysis of nitriles in gold(III) complexes: The structure of [EtC(OEt)NH2]+[AuCl4]â^'. Polyhedron, 1991, 10, 1631-1637.	1.0	18
156	Atmospheric chemistry of FCOxradicals: Kinetic and mechanistic study of the FC(O)O2+ NO2reaction. International Journal of Chemical Kinetics, 1995, 27, 391-402.	1.0	18
157	CF₃CFHO^{â€¢} radical: Decomposition vs. reaction with O₂. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1998, 102, 1850-1856.	0.9	18
158	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
159	Influence of Î±-alumina supports on oxygen binding to Pd, Ag, Pt, and Au. Chemical Physics Letters, 2010, 484, 231-236.	1.2	17
160	Trends in Atomic Adsorption on Pt₃M(111) Transition Metal Bimetallic Surface Overlayers. Journal of Physical Chemistry C, 2014, 118, 8342-8349.	1.5	16
161	Kinetics and mechanism of the gas phase reaction of chlorine atoms with i-propanol. Physical Chemistry Chemical Physics, 2007, 9, 4211.	1.3	15
162	Differences Between Thermal and Laser-Induced Diffusion. Physical Review Letters, 2015, 114, 146104.	2.9	15

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163	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
164	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
165	Electronic structure of asymmetric metal-metal multiple bonds: the d2-d6 molybdenum phosphine-alkoxide complexes X4Mo-Mo(Ph3)4 (X = OH, Cl). Inorganic Chemistry, 1989, 28, 3292-3296.	1.9	13
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