William F Schneider

List of Publications by Citations

212 papers	12,162 citations	55 h-index	103 g-index
232 ext. papers	13,898 ext. citations	6.9 avg, IF	6.53 L-index

#	Paper	IF	Citations
212	Beyond fossil fuel-driven nitrogen transformations. *Science*, **2018**, 360,	33.3	772
211	Equimolar CO(2) absorption by anion-functionalized ionic liquids. *Journal of the American Chemical Society*, **2010**, 132, 2116-7	16.4	689
210	Dynamic multinuclear sites formed by mobilized copper ions in NO selective catalytic reduction. *Science*, **2017**, 357, 898-903	33.3	458
209	The chemistry of water on alumina surfaces: reaction dynamics from first principles. *Science*, **1998**, 282, 265-8	33.3	446
208	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, 6028-48	16.4	405
207	Molecular Design of High Capacity, Low Viscosity, Chemically Tunable Ionic Liquids for CO2 Capture. *Journal of Physical Chemistry Letters*, **2010**, 1, 3494-3499	6.4	335
206	Critical review of Pd-based catalytic treatment of priority contaminants in water. *Environmental Science & Technology*, **2012**, 46, 3655-70	10.3	287
205	Rationalizing the light-induced phase separation of mixed halide organic-inorganic perovskites. *Nature Communications*, **2017**, 8, 200	17.4	264
204	Tracking Iodide and Bromide Ion Segregation in Mixed Halide Lead Perovskites during Photoirradiation. *ACS Energy Letters*, **2016**, 1, 290-296	20.1	251
203	Identification of the active Cu site in standard selective catalytic reduction with ammonia on Cu-SSZ-13. *Journal of Catalysis*, **2014**, 312, 87-97	7.3	247
202	Isolation of the copper redox steps in the standard selective catalytic reduction on Cu-SSZ-13. *Angewandte Chemie - International Edition*, **2014**, 53, 11828-33	16.4	245
201	Density Functional Theory Comparison of Water Dissociation Steps on Cu, Au, Ni, Pd, and Pt. *Journal of Physical Chemistry C*, **2009**, 113, 7269-7276	3.8	220
200	Overcoming ammonia synthesis scaling relations with plasma-enabled catalysis. *Nature Catalysis*, **2018**, 1, 269-275	36.5	193
199	Integrated operando X-ray absorption and DFT characterization of Cu□SZ-13 exchange sites during the selective catalytic reduction of NOx with NH3. *Catalysis Today*, **2012**, 184, 129-144	5.3	187
198	First-Principles Molecular Dynamics Simulations of H2O on □Al2O3 (0001). *Journal of Physical Chemistry B*, **2000**, 104, 5527-5540	3.4	187
197	Chemically tunable ionic liquids with aprotic heterocyclic anion (AHA) for CO(2) capture. *Journal of Physical Chemistry B*, **2014**, 118, 5740-51	3.4	176
196	Thermodynamics of Environment-Dependent Oxygen Chemisorption on Pt(111)□ *Journal of Physical Chemistry C*, **2008**, 112, 9559-9572	3.8	160

195	The Stratospheric Fate of CF3OH. *Environmental Science & Technology*, **1994**, 28, 1198-200	10.3	158
194	The 2020 plasma catalysis roadmap. *Journal Physics D: Applied Physics*, **2020**, 53, 443001	3	141
193	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	3.4	138
192	NO oxidation: A probe reaction on Cu-SSZ-13. *Journal of Catalysis*, **2014**, 312, 179-190	7.3	133
191	Accurate coverage-dependence incorporated into first-principles kinetic models: Catalytic NO oxidation on Pt (111). *Journal of Catalysis*, **2012**, 286, 88-94	7.3	125
190	Catalysis Enabled by Plasma Activation of Strong Chemical Bonds: A Review. *ACS Energy Letters*, **2019**, 4, 1115-1133	20.1	111
189	Atmospheric Chemistry of HFE-7100 (C4F9OCH3): Reaction with OH Radicals, UV Spectra and Kinetic Data for C4F9OCH2• and C4F9OCH2O2• Radicals, and the Atmospheric Fate of C4F9OCH2O• Radicals. *Journal of Physical Chemistry A*, **1997**, 101, 8264-8274	2.8	110
188	Oxygen-coverage effects on molecular dissociations at a Pt metal surface. *Physical Review Letters*, **2009**, 102, 076101	7.4	94
187	Atmospheric Chemistry of the Phenoxy Radical, C6H5O(•): UV Spectrum and Kinetics of Its Reaction with NO, NO2, and O2. *Journal of Physical Chemistry A*, **1998**, 102, 7964-7974	2.8	91
186	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	7.3	86
185	DFT comparison of intrinsic WGS kinetics over Pd and Pt. *Journal of Catalysis*, **2014**, 320, 106-117	7.3	84
184	Cluster Models of Cu Binding and CO and NO Adsorption in Cu-Exchanged Zeolites. *The Journal of Physical Chemistry*, **1996**, 100, 6032-6046		83
183	The environmental impact of CFC replacements - HFCs and HCFCs. *Environmental Science & Technology*, **1994**, 28, 320A-326A	10.3	82
182	Performance of Cluster Expansions of Coverage-Dependent Adsorption of Atomic Oxygen on Pt(111). *Journal of Chemical Theory and Computation*, **2012**, 8, 264-73	6.4	79
181	Catalytic Hydrogenation of CO2 to Formic Acid with Silica-Tethered Iridium Catalysts. *ChemCatChem*, **2013**, 5, 1769-1771	5.2	79
180	Density Functional Theory Study of Transformations of Nitrogen Oxides Catalyzed by Cu-Exchanged Zeolites. *Journal of Physical Chemistry B*, **1998**, 102, 3692-3705	3.4	79
179	Progress in Accurate Chemical Kinetic Modeling, Simulations, and Parameter Estimation for Heterogeneous Catalysis. *ACS Catalysis*, **2019**, 9, 6624-6647	13.1	78
178	DFT-Based Coverage-Dependent Model of Pt-Catalyzed NO Oxidation. *ChemCatChem*, **2010**, 2, 1450-1460	5.2	77

177	DFT-Based Characterization of the Multiple Adsorption Modes of Nitrogen Oxides on Pt(111). *Journal of Physical Chemistry C*, **2007**, 111, 389-397	3.8	76
176	Dramatic Cooperative Effects in Adsorption of NOx on MgO(001). *Journal of Physical Chemistry B*, **2002**, 106, 7405-7413	3.4	75
175	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	21.8	74
174	Kinetics and Mechanisms of the Self-Reactions of CCl3O2 and CHCl2O2 Radicals and Their Reactions with HO2. *The Journal of Physical Chemistry*, **1996**, 100, 14356-14371		73
173	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	5.3	71
172	First-principles-guided design of ionic liquids for CO2 capture. *Physical Chemistry Chemical Physics*, **2012**, 14, 13163-70	3.6	70
171	Combined Computational and Experimental Investigation of SOx Adsorption on MgO. *Journal of Physical Chemistry B*, **2001**, 105, 6972-6979	3.4	66
170	Experimental and Computational Investigation of Effect of Sr on NO Oxidation and Oxygen Exchange for La1−xSrxCoO3 Perovskite Catalysts. *ACS Catalysis*, **2013**, 3, 2719-2728	13.1	64
169	DFT Investigation of Intermediate Steps in the Hydrolysis of α-Al2O3(0001). *Journal of Physical Chemistry C*, **2009**, 113, 2149-2158	3.8	63
168	DFT characterization of coverage dependent molecular water adsorption modes on α-Al2O3(0 0 0 1). *Surface Science*, **2008**, 602, 268-275	1.8	63
167	NO oxidation properties of Pt(111) revealed by ab initio kinetic simulations. *Physical Review B*, **2005** , 71,	3.3	63
166	Structure Sensitivity Study of Waterborne Contaminant Hydrogenation Using Shape- and Size-Controlled Pd Nanoparticles. *ACS Catalysis*, **2013**, 3, 453-463	13.1	62
165	Effect of particle size on the oxidizability of platinum clusters. *Journal of Physical Chemistry A*, **2006**, 110, 5839-46	2.8	62
164	Effect of Particle Size on the Adsorption of O and S Atoms on Pt: A Density-Functional Theory Study. *Journal of Physical Chemistry B*, **2001**, 105, 7739-7747	3.4	62
163	Influence of dipole-dipole interactions on coverage-dependent adsorption: CO and NO on Pt(111). *Langmuir*, **2012**, 28, 8408-17	4	58
162	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	3.4	58
161	Distinguishing Plasma Contributions to Catalyst Performance in Plasma-Assisted Ammonia Synthesis. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 8621-8630	8.3	55
160	Theoretical analysis of oxygen-bridged Cu pairs in Cu-exchanged zeolites. *Catalysis Letters*, **1998**, 56, 183-188	2.8	55

159	Chemistry of Sulfur Oxides on Transition Metals I: Configurations, Energetics, Orbital Analyses, and Surface Coverage Effects of SO2on Pt(111). *Journal of Physical Chemistry B*, **2002**, 106, 12575-12583	3.4	55
158	Ab initio investigation of the heats of formation of several trifluoromethyl compounds. *The Journal of Physical Chemistry*, **1993**, 97, 12783-12788		55
157	Cluster Model Studies of Oxygen-Bridged Cu Pairs in Cu ZSM-5 Catalysts. *Journal of Physical Chemistry B*, **1999**, 103, 10452-10460	3.4	54
156	Hydrofluorocarbons and stratospheric ozone. *Faraday Discussions*, **1995**, 100, 55	3.6	54
155	Consequences of exchange-site heterogeneity and dynamics on the UV-visible spectrum of Cu-exchanged SSZ-13. *Chemical Science*, **2019**, 10, 2373-2384	9.4	53
154	Bond Strength Trends in Halogenated Methanols: Evidence for Negative Hyperconjugation?. *Journal of the American Chemical Society*, **1995**, 117, 478-485	16.4	53
153	Intermediates and Spectators in O2 Dissociation at the RuO2(110) Surface. *Journal of Physical Chemistry C*, **2009**, 113, 15266-15273	3.8	50
152	CO2 Chemistry of Phenolate-Based Ionic Liquids. *Journal of Physical Chemistry B*, **2016**, 120, 1509-17	3.4	49
151	How low can you go? Minimum energy pathways for O2 dissociation on Pt(111). *Physical Chemistry Chemical Physics*, **2012**, 14, 16677-85	3.6	48
150	Computational comparison of the reactions of substituted amines with CO(2). *ChemSusChem*, **2010**, 3, 931-8	8.3	48
149	Cu Dinitrosyl Species in Zeolites: A Density Functional Molecular Cluster Study. *Journal of Physical Chemistry B*, **1997**, 101, 6903-6913	3.4	48
148	Atmospheric chemistry of CH3Cl: mechanistic study of the reaction of CH2ClO2 radicals with HO2. *Chemical Physics Letters*, **1996**, 251, 164-173	2.5	48
147	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	16.4	47
146	Role of Molecular Modeling in the Development of CO-Reactive Ionic Liquids. *Chemical Reviews*, **2018**, 118, 5242-5260	68.1	47
145	Competing reactions of CO2 with cations and anions in azolide ionic liquids. *ChemSusChem*, **2014**, 7, 1970-5	8.3	47
144	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, 4125-33	2.8	47
143	Comparison of Explicit and United Atom Models for Alkane Chains Physisorbed on Al2O3 (0001). *Journal of Physical Chemistry B*, **1999**, 103, 3885-3895	3.4	47
142	Atmospheric chemistry of trifluoromethoxy radicals: reaction with water. *The Journal of Physical Chemistry*, **1993**, 97, 7606-7611		45

141	Implications of coverage-dependent O adsorption for catalytic NO oxidation on the late transition metals. *Catalysis Science and Technology*, **2014**, 4, 4356-4365	5.5	44
140	Thermodynamic equilibrium compositions, structures, and reaction energies of Pt(x)O(y) (x = 1-3) clusters predicted from first principles. *Journal of Physical Chemistry B*, **2006**, 110, 16591-9	3.4	44
139	Formation of methane sulfinic acid in the gas-phase OH-radical initiated oxidation of dimethyl sulfoxide. *Environmental Science & Technology*, **2002**, 36, 5155-63	10.3	43
138	Stability and infrared spectra of mono-, di-, and trichloromethanol. *Chemical Physics Letters*, **2000**, 322, 97-102	2.5	43
137	Reliability of Small Cluster Models for Cu-Exchanged Zeolites. *The Journal of Physical Chemistry*, **1996**, 100, 9292-9301		43
136	Energetics and Mechanism of Decomposition of CF3OH. *The Journal of Physical Chemistry*, **1996**, 100, 6097-6103		42
135	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, 6009-18	3.6	42
134	First-Principles Characterization of NOx Adsorption on MgO. *Journal of Physical Chemistry B*, **2003**, 107, 157-163	3.4	42
133	Mechanistic study of the gas-phase reaction of CH2FO2 radicals with HO2. *Chemical Physics Letters*, **1994**, 218, 34-42	2.5	42
132	Effects of coverage on the structures, energetics, and electronics of oxygen adsorption on RuO2(110). *Journal of Chemical Physics*, **2007**, 127, 064706	3.9	41
131	Adsorption Energy Correlations at the Metal–Support Boundary. *ACS Catalysis*, **2017**, 7, 4707-4715	13.1	40
130	Plasma-Catalytic Ammonia Synthesis beyond the Equilibrium Limit. *ACS Catalysis*, **2020**, 10, 6726-6734	13.1	40
129	Chemistry of Sulfur Oxides on Transition Metals. II. Thermodynamics of Sulfur Oxides on Platinum(111). *Journal of Physical Chemistry B*, **2004**, 108, 250-264	3.4	40
128	Statistical analysis of Al distributions and metal ion pairing probabilities in zeolites. *Catalysis Letters* , **2000**, 68, 85-93	2.8	40
127	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		40
126	Experimental and Computational Interrogation of Fast SCR Mechanism and Active Sites on H-Form SSZ-13. *ACS Catalysis*, **2017**, 7, 5087-5096	13.1	39
125	Chemistry of Sulfur Oxides on Transition Metals. III. Oxidation of SO2 and Self-Diffusion of O, SO2, and SO3 on Pt(111). *Journal of Physical Chemistry B*, **2004**, 108, 13329-13340	3.4	39
124	Catalysis Science of NOx Selective Catalytic Reduction With Ammonia Over Cu-SSZ-13 and Cu-SAPO-34. *Advances in Catalysis*, **2016**, 1-107	2.4	38

123	Density functional studies of adsorbates in Cu-exchanged zeolites: model comparisons and SOx binding. *Physical Chemistry Chemical Physics*, **1999**, 1, 639-648	3.6	38
122	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	24.3	37
121	DFT Analysis of NO Oxidation Intermediates on Undoped and Doped LaCoO3 Perovskite. *Journal of Physical Chemistry C*, **2015**, 119, 20488-20494	3.8	36
120	Zeolite Adsorption Free Energies from ab Initio Potentials of Mean Force. *Journal of Chemical Theory and Computation*, **2018**, 14, 929-938	6.4	36
119	Development and application of effective pairwise potentials for UO2(n+), NpO2(n+), PuO2(n+), and AmO2(n+) (n = 1, 2) ions with water. *Physical Chemistry Chemical Physics*, **2013**, 15, 15954-63	3.6	35
118	Isolation of the Copper Redox Steps in the Standard Selective Catalytic Reduction on Cu-SSZ-13. *Angewandte Chemie*, **2014**, 126, 12022-12027	3.6	35
117	Ordering and Oxygen Adsorption in Au$_x$Pt/Pt(111) Surface Alloys. *Journal of Physical Chemistry C*, **2011**, 115, 17915-17924	3.8	35
116	Simulations of hydrocarbon adsorption and subsequent water penetration on an aluminum oxide surface. *Journal of Chemical Physics*, **1997**, 106, 7331-7342	3.9	35
115	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	3	34
114	Potential energy surfaces for oxygen adsorption, dissociation, and diffusion at the Pt(321) surface. *Langmuir*, **2011**, 27, 8177-86	4	34
113	Direct control of electron transfer to the surface-CO bond on a Pt/TiO2 catalytic diode. *Journal of the American Chemical Society*, **2011**, 133, 16459-67	16.4	34
112	Thermal decomposition of dispersed and bulk-like NOx species in model NOx trap materials. *Applied Catalysis B: Environmental*, **2005**, 61, 164-175	21.8	34
111	Theoretical Study of CO and NO Vibrational Frequencies in Cu$_n$Water Clusters and Implications for Cu-Exchanged Zeolites. *Journal of Physical Chemistry B*, **1997**, 101, 1940-1949	3.4	33
110	Thermochemistry of COF2 and Related Compounds. *The Journal of Physical Chemistry*, **1994**, 98, 7448-7451		33
109	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	5.1	33
108	First-Principles Analysis of Site- and Condition-Dependent Fe Speciation in SSZ-13 and Implications for Catalyst Optimization. *ACS Catalysis*, **2018**, 8, 10119-10130	13.1	33
107	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, 10852-68	3.4	32
106	Benchmark First-Principles Calculations of Adsorbate Free Energies. *ACS Catalysis*, **2018**, 8, 1945-1954	13.1	31

105	Structure- and Temperature-Dependence of Pt-Catalyzed Ammonia Oxidation Rates and Selectivities. *ACS Catalysis*, **2019**, 9, 2407-2414	13.1	30
104	Comparison of cluster expansion fitting algorithms for interactions at surfaces. *Surface Science*, **2015**, 640, 104-111	1.8	30
103	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	6.4	30
102	Enhancement of oxyanion and diatrizoate reduction kinetics using selected azo dyes on Pd-based catalysts. *Environmental Science & Technology*, **2010**, 44, 1773-9	10.3	30
101	First-Principles Analysis of Structure Sensitivity in NO Oxidation on Pt. *ACS Catalysis*, **2015**, 5, 1087-1099	13.1	29
100	Kinetic study of the reaction CF3O+O3-CF3O2+O2. *Chemical Physics Letters*, **1993**, 213, 442-448	2.5	29
99	The Environmental Impact of CFC Replacements HFCs and HCFCs. *Environmental Science & Technology*, **1994**, 28, 320A-6A	10.3	28
98	Structure and bonding trends in two- and three-coordinate boron cations. *Inorganic Chemistry*, **1991**, 30, 3919-3927	5.1	28
97	Solid-state covalent capture of CO2 by using N-heterocyclic carbenes. *Chemistry - A European Journal*, **2013**, 19, 11134-8	4.8	27
96	Chemistry for a sustainable future. *Environmental Science & Technology*, **2007**, 41, 4840-6	10.3	27
95	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, 6018-23	3.4	26
94	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	1.4	26
93	Theoretical Analysis of N2O to N2 Conversion During the Catalytic Decomposition of NO by Cu-Zeolites. *Catalysis Letters*, **2001**, 74, 193-199	2.8	26
92	Density functional theory description of excited-state intramolecular proton transfer. *Chemical Physics Letters*, **1996**, 263, 414-422	2.5	26
91	Effects of dioxygen pressure on rates of NOx selective catalytic reduction with NH3 on Cu-CHA zeolites. *Journal of Catalysis*, **2020**, 389, 140-149	7.3	25
90	Ion Transport in Solvent-Free, Crosslinked, Single-Ion Conducting Polymer Electrolytes for Post-Lithium Ion Batteries. *Batteries*, **2018**, 4, 28	5.7	25
89	Novel Structural Modifications Associated with the Highly Efficient Internal Conversion of 2-(2□Hydroxyphenyl)benzotriazole Ultraviolet Stabilizers. *Journal of the American Chemical Society*, **1997**, 119, 5445-5446	16.4	25
88	Surface termination effects on metal atom adsorption on □alumina. *Surface Science*, **2008**, 602, 3445-3453	2.8	25

87	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	3.8	25
86	Interplay between subsurface ordering, surface segregation, and adsorption on Pt-Ti(111) near-surface alloys. *Langmuir*, **2012**, 28, 4683-93	4	24
85	Nature and role of surface carbonates and bicarbonates in CO oxidation over RuO(2). *Physical Chemistry Chemical Physics*, **2010**, 12, 6367-74	3.6	24
84	First-principles reaction site model for coverage-sensitive surface reactions: Pt(111)□O temperature programmed desorption. *Surface Science*, **2014**, 622, L1-L6	1.8	23
83	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	2.3	23
82	Periodic DFT Characterization of NOx Adsorption in Cu-Exchanged SSZ-13 Zeolite Catalysts. *Journal of Physical Chemistry C*, **2016**, 120, 27934-27943	3.8	22
81	First-principles cluster expansion study of missing-row reconstructions of fcc (110) surfaces. *Physical Review B*, **2011**, 83,	3.3	22
80	Molecular Origins of Selectivity in the Reduction of NOxby NH3. *Journal of Physical Chemistry A*, **2004**, 108, 9365-9374	2.8	22
79	Atmospheric Chemistry of CF3OH: Is Photolysis Important?. *Environmental Science & Technology*, **1995**, 29, 247-50	10.3	22
78	LDA+U evaluation of the stability of low-index facets of LaCoO3 perovskite. *Surface Science*, **2014**, 619, 71-76	1.8	21
77	Site specific carboxylation of abnormal anionic N-heterocyclic dicarbenes with CO2. *Chemical Communications*, **2013**, 49, 11527-9	5.8	21
76	Adsorption and reactions of NOx on RuO2(1 1 0). *Catalysis Today*, **2011**, 165, 49-55	5.3	21
75	Kinetics and mechanism of the reaction of Cl atoms with CH2 CO (Ketene). *International Journal of Chemical Kinetics*, **1996**, 28, 627-635	1.4	21
74	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	21.8	20
73	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		20
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71	The vibrational spectrum of FC(O)O radical: A challenging case for single-reference electron correlation methods. *Journal of Chemical Physics*, **1995**, 103, 6601-6607	3.9	19
70	Predicted Influence of Plasma Activation on Nonoxidative Coupling of Methane on Transition Metal Catalysts. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 6043-6054	8.3	18

69	CF3CFHO□radical: Decomposition vs. reaction with O2. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1998**, 102, 1850-1856		18
68	Characterization of adsorption trends of NO2, nitrite, and nitrate on MgO terraces. *Surface Science*, **2003**, 546, 75-86	1.8	18
67	Atmospheric chemistry of FCOx radicals: Kinetic and mechanistic study of the FC(O)O2 + NO2 reaction. *International Journal of Chemical Kinetics*, **1995**, 27, 391-402	1.4	17
66	Atomic-Scale Structural Evolution of Rh(110) during Catalysis. *ACS Catalysis*, **2017**, 7, 664-674	13.1	16
65	Influence of □alumina supports on oxygen binding to Pd, Ag, Pt, and Au. *Chemical Physics Letters*, **2010**, 484, 231-236	2.5	16
64	Alcoholysis of nitriles in gold(III) complexes: The structure of [EtC(OEt)NH2]+[AuCl4]□*Polyhedron*, **1991**, 10, 1631-1637	2.7	16
63	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	3.4	15
62	Evaluation of ionic fluids as lubricants in manufacturing. *Journal of Manufacturing Processes*, **2013**, 15, 414-418	5	15
61	Band structure of germanium carbides for direct bandgap silicon photonics. *Journal of Applied Physics*, **2016**, 120, 053102	2.5	15
60	DFT and microkinetic comparison of Pt, Pd and Rh-catalyzed ammonia oxidation. *Journal of Catalysis*, **2020**, 383, 322-330	7.3	14
59	Participation of interfacial hydroxyl groups in the water-gas shift reaction over Au/MgO catalysts. *Catalysis Science and Technology*, **2017**, 7, 5257-5266	5.5	14
58	Kinetics and mechanism of the gas phase reaction of chlorine atoms with i-propanol. *Physical Chemistry Chemical Physics*, **2007**, 9, 4211-7	3.6	14
57	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	3.8	12
56	Differences between thermal and laser-induced diffusion. *Physical Review Letters*, **2015**, 114, 146104	7.4	12
55	Trends in Atomic Adsorption on Pt3M(111) Transition Metal Bimetallic Surface Overlayers. *Journal of Physical Chemistry C*, **2014**, 118, 8342-8349	3.8	12
54	Molecular origins of surface poisoning during CO oxidation over RuO2(1 1 0). *Surface Science*, **2009**, 603, L91-L94	1.8	12
53	Kinetics of Elementary Reactions in the Chain Chlorination of Cyclopropane. *Journal of Physical Chemistry A*, **2003**, 107, 2003-2010	2.8	12
52	Atmospheric chemistry of HFC-134a. Kinetic and mechanistic study of the CF3CFHO2+NO2 reaction. *Chemical Physics Letters*, **1994**, 225, 375-380	2.5	11

51	Comparison of Coverage-Dependent Binding Energy Models for Mean-Field Microkinetic Rate Predictions. *Langmuir*, **2020**, 36, 465-474	4	11
50	Comparative chemistries of CO and NO oxidation over RuO2(110): insights from first-principles thermodynamics and kinetics. *Molecular Simulation*, **2012**, 38, 615-630	2	10
49	Aqueous N2O Reduction with H2 Over Pd-Based Catalyst: Mechanistic Insights From Experiment and Simulation. *Topics in Catalysis*, **2012**, 55, 300-312	2.3	10
48	Computational Comparison of Tethering Strategies for Amine Functionalised Ionic Liquids. *ACS Symposium Series*, **2010**, 419-430	0.4	10
47	Reply to "Comment on the Thermochemistry of the CF3O Radical and CF3OH". *The Journal of Physical Chemistry*, **1994**, 98, 2217-2218		10
46	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	5.1	10
45	Effects of Brønsted acid site proximity in chabazite zeolites on OH infrared spectra and protolytic propane cracking kinetics. *Journal of Catalysis*, **2021**, 395, 210-226	7.3	10
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