William F Schneider

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Consequences of adsorbate-adsorbate interactions for apparent kinetics of surface catalytic reactions. *Journal of Catalysis*, **2022**, 405, 410-418	7.3	1
211	Observation and rationalization of nitrogen oxidation enabled only by coupled plasma and catalyst.. *Nature Communications*, **2022**, 13, 402	17.4	1
210	CO and C3H6 poisoning of hydrogen permeation across Pd77Ag23 alloy membranes: A comparative study with pure palladium. *Chemical Engineering Journal*, **2022**, 430, 133080	14.7	2
209	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
208	Inelastic Neutron Scattering Observation of Plasma-Promoted Nitrogen Reduction Intermediates on Ni/γ-Al2O3. *ACS Energy Letters*, **2021**, 6, 2048-2053	20.1	3
207	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	3.8	0
206	Plasma-catalyst modeling for materials selection: challenges and opportunities in nitrogen oxidation. *Journal Physics D: Applied Physics*, **2021**, 54, 454004	3	1
205	Adsorbate Free Energies from DFT-Derived Translational Energy Landscapes. *Journal of Physical Chemistry C*, **2021**, 125, 20331-20342	3.8	3
204	Plasma-Catalytic Ammonia Synthesis beyond the Equilibrium Limit. *ACS Catalysis*, **2020**, 10, 6726-6734	13.1	40
203	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
202	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	3.9	7
201	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
200	DFT and microkinetic comparison of Pt, Pd and Rh-catalyzed ammonia oxidation. *Journal of Catalysis*, **2020**, 383, 322-330	7.3	14
199	Characteristics of Impactful Computational Contributions to The Journal of Physical Chemistry C. *Journal of Physical Chemistry C*, **2020**, 124, 13509-13510	3.8	3
198	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
197	Supercell Models of Brønsted and Lewis Sites in Zeolites **2020**, 1355-1375		1
196	The 2020 plasma catalysis roadmap. *Journal Physics D: Applied Physics*, **2020**, 53, 443001	3	141

195	Comparison of Coverage-Dependent Binding Energy Models for Mean-Field Microkinetic Rate Predictions. *Langmuir*, **2020**, 36, 465-474	4	11
194	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
193	Structure- and Temperature-Dependence of Pt-Catalyzed Ammonia Oxidation Rates and Selectivities. *ACS Catalysis*, **2019**, 9, 2407-2414	13.1	30
192	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
191	Water-Mediated Reduction of Aqueous N-Nitrosodimethylamine with Pd. *Environmental Science & Technology*, **2019**, 53, 7551-7563	10.3	7
190	Progress in Accurate Chemical Kinetic Modeling, Simulations, and Parameter Estimation for Heterogeneous Catalysis. *ACS Catalysis*, **2019**, 9, 6624-6647	13.1	78
189	Distinguishing Plasma Contributions to Catalyst Performance in Plasma-Assisted Ammonia Synthesis. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 8621-8630	8.3	55
188	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
187	Catalysis Enabled by Plasma Activation of Strong Chemical Bonds: A Review. *ACS Energy Letters*, **2019**, 4, 1115-1133	20.1	111
186	The Periodic Table. *Journal of Physical Chemistry A*, **2019**, 123, 5837-5848	2.8	1
185	The JPC Periodic Table. *Journal of Physical Chemistry C*, **2019**, 123, 17063-17074	3.8	1
184	The JPC Periodic Table. *Journal of Physical Chemistry Letters*, **2019**, 10, 4051-4062	6.4	1
183	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
182	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
181	Role of Molecular Modeling in the Development of CO-Reactive Ionic Liquids. *Chemical Reviews*, **2018**, 118, 5242-5260	68.1	47
180	Machine Learning. *Journal of Physical Chemistry A*, **2018**, 122, 879	2.8	5
179	Machine Learning. *Journal of Physical Chemistry B*, **2018**, 122, 1347	3.4	2
178	Machine Learning. *Journal of Physical Chemistry Letters*, **2018**, 9, 569	6.4	3

177	Benchmark First-Principles Calculations of Adsorbate Free Energies. *ACS Catalysis*, **2018**, 8, 1945-1954	13.1	31
176	Overcoming ammonia synthesis scaling relations with plasma-enabled catalysis. *Nature Catalysis*, **2018**, 1, 269-275	36.5	193
175	Ion Transport in Solvent-Free, Crosslinked, Single-Ion Conducting Polymer Electrolytes for Post-Lithium Ion Batteries. *Batteries*, **2018**, 4, 28	5.7	25
174	Zeolite Adsorption Free Energies from ab Initio Potentials of Mean Force. *Journal of Chemical Theory and Computation*, **2018**, 14, 929-938	6.4	36
173	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
172	Supercell Models of Br□sted and Lewis Sites in Zeolites **2018**, 1-21		
171	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
170	Beyond fossil fuel-driven nitrogen transformations. *Science*, **2018**, 360,	33.3	772
169	Hybrid Computational Strategy for Predicting CO2 Solubilities in Reactive Ionic Liquids. *Journal of Physical Chemistry C*, **2018**, 122, 14213-14221	3.8	8
168	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
167	Adsorption Energy Correlations at the Metal□Support Boundary. *ACS Catalysis*, **2017**, 7, 4707-4715	13.1	40
166	Binary Approach to Ternary Cluster Expansions: NO□□Vacancy System on Pt(111). *Journal of Physical Chemistry C*, **2017**, 121, 7344-7354	3.8	19
165	Atomic-Scale Structural Evolution of Rh(110) during Catalysis. *ACS Catalysis*, **2017**, 7, 664-674	13.1	16
164	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
163	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
162	New Physical Insights from a Computational Catalysis Perspective. *Journal of Physical Chemistry C*, **2017**, 121, 15491-15492	3.8	1
161	Rationalizing the light-induced phase separation of mixed halide organic-inorganic perovskites. *Nature Communications*, **2017**, 8, 200	17.4	264
160	Dynamic multinuclear sites formed by mobilized copper ions in NO selective catalytic reduction. *Science*, **2017**, 357, 898-903	33.3	458

159	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
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	3.4	15
157	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
156	Tracking Iodide and Bromide Ion Segregation in Mixed Halide Lead Perovskites during Photoirradiation. *ACS Energy Letters*, **2016**, 1, 290-296	20.1	251
155	CO2 Chemistry of Phenolate-Based Ionic Liquids. *Journal of Physical Chemistry B*, **2016**, 120, 1509-17	3.4	49
154	Band structure of germanium carbides for direct bandgap silicon photonics. *Journal of Applied Physics*, **2016**, 120, 053102	2.5	15
153	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
152	Band Anticrossing in Dilute Germanium Carbides Using Hybrid Density Functionals. *Journal of Electronic Materials*, **2016**, 45, 2121-2126	1.9	4
151	Comparison of cluster expansion fitting algorithms for interactions at surfaces. *Surface Science*, **2015**, 640, 104-111	1.8	30
150	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
149	Differences between thermal and laser-induced diffusion. *Physical Review Letters*, **2015**, 114, 146104	7.4	12
148	DFT Analysis of NO Oxidation Intermediates on Undoped and Doped LaCoO3 Perovskite. *Journal of Physical Chemistry C*, **2015**, 119, 20488-20494	3.8	36
147	First-Principles Analysis of Structure Sensitivity in NO Oxidation on Pt. *ACS Catalysis*, **2015**, 5, 1087-1099	13.1	29
146	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
145	NO oxidation: A probe reaction on Cu-SSZ-13. *Journal of Catalysis*, **2014**, 312, 179-190	7.3	133
144	First-principles reaction site model for coverage-sensitive surface reactions: Pt(111)D temperature programmed desorption. *Surface Science*, **2014**, 622, L1-L6	1.8	23
143	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
142	DFT comparison of intrinsic WGS kinetics over Pd and Pt. *Journal of Catalysis*, **2014**, 320, 106-117	7.3	84

141	Trends in Atomic Adsorption on Pt3M(111) Transition Metal Bimetallic Surface Overlayers. *Journal of Physical Chemistry C*, **2014**, 118, 8342-8349	3.8	12
140	Competing reactions of CO2 with cations and anions in azolide ionic liquids. *ChemSusChem*, **2014**, 7, 1978-85	8.5	47
139	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
138	LDA+U evaluation of the stability of low-index facets of LaCoO3 perovskite. *Surface Science*, **2014**, 619, 71-76	1.8	21
137	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
136	Performance implications of chemical absorption for the carbon-dioxide-cofluid refrigeration cycle. *International Journal of Refrigeration*, **2014**, 46, 196-206	3.8	9
135	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
134	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
133	Solid-state covalent capture of CO2 by using N-heterocyclic carbenes. *Chemistry - A European Journal*, **2013**, 19, 11134-8	4.8	27
132	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
131	Structure Sensitivity Study of Waterborne Contaminant Hydrogenation Using Shape- and Size-Controlled Pd Nanoparticles. *ACS Catalysis*, **2013**, 3, 453-463	13.1	62
130	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
129	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
128	Site specific carboxylation of abnormal anionic N-heterocyclic dicarbenes with CO2. *Chemical Communications*, **2013**, 49, 11527-9	5.8	21
127	Evaluation of ionic fluids as lubricants in manufacturing. *Journal of Manufacturing Processes*, **2013**, 15, 414-418	5	15
126	Catalytic Hydrogenation of CO2 to Formic Acid with Silica-Tethered Iridium Catalysts. *ChemCatChem*, **2013**, 5, 1769-1771	5.2	79
125	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
124	First-principles-guided design of ionic liquids for CO2 capture. *Physical Chemistry Chemical Physics*, **2012**, 14, 13163-70	3.6	70

123	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
122	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
121	Interplay between subsurface ordering, surface segregation, and adsorption on Pt-Ti(111) near-surface alloys. *Langmuir*, **2012**, 28, 4683-93	4	24
120	Influence of dipole-dipole interactions on coverage-dependent adsorption: CO and NO on Pt(111). *Langmuir*, **2012**, 28, 8408-17	4	58
119	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	1.8	6
118	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
117	Critical review of Pd-based catalytic treatment of priority contaminants in water. *Environmental Science & Technology*, **2012**, 46, 3655-70	10.3	287
116	Response to Comment on Critical Review of Pd-Based Catalytic Treatment of Priority Contaminants in Water *Environmental Science & Technology*, **2012**, 46, 11469-11470	10.3	9
115	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
114	Integrated operando X-ray absorption and DFT characterization of Cu SSZ-13 exchange sites during the selective catalytic reduction of NOx with NH3. *Catalysis Today*, **2012**, 184, 129-144	5.3	187
113	Ordering and Oxygen Adsorption in Au Pt/Pt(111) Surface Alloys. *Journal of Physical Chemistry C*, **2011**, 115, 17915-17924	3.8	35
112	Potential energy surfaces for oxygen adsorption, dissociation, and diffusion at the Pt(321) surface. *Langmuir*, **2011**, 27, 8177-86	4	34
111	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
110	First-principles cluster expansion study of missing-row reconstructions of fcc (110) surfaces. *Physical Review B*, **2011**, 83,	3.3	22
109	DFT Comparison of N-Nitrosodimethylamine Decomposition Pathways Over Ni and Pd. *ChemCatChem*, **2011**, 3, 898-903	5.2	9
108	Adsorption and reactions of NOx on RuO2(1 1 0). *Catalysis Today*, **2011**, 165, 49-55	5.3	21
107	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
106	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

105	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
104	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
103	DFT-Based Coverage-Dependent Model of Pt-Catalyzed NO Oxidation. *ChemCatChem*, **2010**, 2, 1450-1460	5.2	77
102	Computational Comparison of Tethering Strategies for Amine Functionalised Ionic Liquids. *ACS Symposium Series*, **2010**, 419-430	0.4	10
101	Equimolar CO(2) absorption by anion-functionalized ionic liquids. *Journal of the American Chemical Society*, **2010**, 132, 2116-7	16.4	689
100	Computational comparison of the reactions of substituted amines with CO(2). *ChemSusChem*, **2010**, 3, 931-8	8.3	48
99	Influence of □alumina supports on oxygen binding to Pd, Ag, Pt, and Au. *Chemical Physics Letters*, **2010**, 484, 231-236	2.5	16
98	Molecular origins of surface poisoning during CO oxidation over RuO2(1 1 0). *Surface Science*, **2009**, 603, L91-L94	1.8	12
97	Oxygen-coverage effects on molecular dissociations at a Pt metal surface. *Physical Review Letters*, **2009**, 102, 076101	7.4	94
96	Intermediates and Spectators in O2 Dissociation at the RuO2(110) Surface. *Journal of Physical Chemistry C*, **2009**, 113, 15266-15273	3.8	50
95	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
94	DFT Investigation of Intermediate Steps in the Hydrolysis of □Al2O3(0001)□ *Journal of Physical Chemistry C*, **2009**, 113, 2149-2158	3.8	63
93	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
92	Thermodynamics of Environment-Dependent Oxygen Chemisorption on Pt(111)□ *Journal of Physical Chemistry C*, **2008**, 112, 9559-9572	3.8	160
91	Experimental and computational investigation of gas-phase reaction of chlorine with n-propanol: observation of chloropropanol conformational isomerization at room temperature. *Journal of Physical Chemistry A*, **2008**, 112, 2773-81	2.8	8
90	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
89	DFT characterization of coverage dependent molecular water adsorption modes on □Al2O3(0 0 0 1). *Surface Science*, **2008**, 602, 268-275	1.8	63
88	Surface termination effects on metal atom adsorption on □alumina. *Surface Science*, **2008**, 602, 3445-3453	1.8	25

87	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
86	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
85	Chemistry for a sustainable future. *Environmental Science & Technology*, **2007**, 41, 4840-6	10.3	27
84	Transferable Force Field for Water Adsorption in Cation-Exchanged Titanosilicates. *Industrial & Engineering Chemistry Research*, **2007**, 46, 5754-5765	3.9	3
83	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
82	Catalysis by Design - Theoretical and Experimental Studies of Model Catalysts **2007**,		2
81	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
80	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
79	Effect of particle size on the oxidizability of platinum clusters. *Journal of Physical Chemistry A*, **2006**, 110, 5839-46	2.8	62
78	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
77	Theoretical Aspects of Oxide Particle Stability and Chemical Reactivity **2006**, 289-309		
76	A thermogravimetric determination of dispersed and bulk-like barium species supported on □alumina. *Journal of Materials Chemistry*, **2005**, 15, 366-368		8
75	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
74	NO oxidation properties of Pt(111) revealed by ab initio kinetic simulations. *Physical Review B*, **2005** , 71,	3.3	63
73	Molecular Origins of Selectivity in the Reduction of NOxby NH3. *Journal of Physical Chemistry A*, **2004**, 108, 9365-9374	2.8	22
72	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
71	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
70	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

69	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	1.4	6
68	Characterization of adsorption trends of NO2, nitrite, and nitrate on MgO terraces. *Surface Science*, **2003**, 546, 75-86	1.8	18
67	First-Principles Characterization of NOx Adsorption on MgO. *Journal of Physical Chemistry B*, **2003**, 107, 157-163	3.4	42
66	Kinetics of Elementary Reactions in the Chain Chlorination of Cyclopropane. *Journal of Physical Chemistry A*, **2003**, 107, 2003-2010	2.8	12
65	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
64	Simulated performance and cofluid dependence of a CO2-cofluid refrigeration cycle with wet compression. *International Journal of Refrigeration*, **2002**, 25, 1123-1136	3.8	8
63	Dramatic Cooperative Effects in Adsorption of NOx on MgO(001). *Journal of Physical Chemistry B*, **2002**, 106, 7405-7413	3.4	75
62	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
61	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
60	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
59	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
58	Combined Computational and Experimental Investigation of SOx Adsorption on MgO. *Journal of Physical Chemistry B*, **2001**, 105, 6972-6979	3.4	66
57	Stability and infrared spectra of mono-, di-, and trichloromethanol. *Chemical Physics Letters*, **2000**, 322, 97-102	2.5	43
56	Statistical analysis of Al distributions and metal ion pairing probabilities in zeolites. *Catalysis Letters* , **2000**, 68, 85-93	2.8	40
55	Cycle-Model Assessment of Working Fluids for a Low-Pressure CO2 Climate Control System **2000**,		4
54	First-Principles Molecular Dynamics Simulations of H2O on Al2O3 (0001). *Journal of Physical Chemistry B*, **2000**, 104, 5527-5540	3.4	187
53	Thermodynamic and Cycle Models for a Low-Pressure CO2 Refrigeration Cycle **1999**,		6
52	CO oxidation catalyzed by Cu-exchanged zeolites: a density functional theory study. *Catalysis Letters*, **1999**, 61, 179-186	2.8	6

51	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
50	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
49	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
48	Theoretical analysis of oxygen-bridged Cu pairs in Cu-exchanged zeolites. *Catalysis Letters*, **1998**, 56, 183-188	2.8	55
47	CF3CFHO□radical: Decomposition vs. reaction with O2. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1998**, 102, 1850-1856		18
46	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
45	The chemistry of water on alumina surfaces: reaction dynamics from first principles. *Science*, **1998**, 282, 265-8	33.3	446
44	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
43	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
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