

# Alexis T Bell

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/5142584/publications.pdf>

Version: 2024-02-01

531  
papers

59,447  
citations

1094

112  
h-index

1341

223  
g-index

560  
all docs

560  
docs citations

560  
times ranked

40452  
citing authors

#	ARTICLE	IF	CITATIONS
1	Membrane-electrode assembly design parameters for optimal CO <sub>2</sub> reduction. <i>Electrochemical Science Advances</i> , 2023, 3, .	1.2	14
2	Insights into the mechanism and kinetics of propene oxidation and ammoxidation over bismuth molybdate catalysts derived from experiments and theory. <i>Journal of Catalysis</i> , 2022, 408, 436-452.	3.1	18
3	Investigation of the modes of NO adsorption in Pd/H-CHA. <i>Applied Catalysis B: Environmental</i> , 2022, 304, 120992.	10.8	18
4	Mechanistic understanding of pH effects on the oxygen evolution reaction. <i>Electrochimica Acta</i> , 2022, 405, 139810.	2.6	31
5	Engineering Catalyst-Electrolyte Microenvironments to Optimize the Activity and Selectivity for the Electrochemical Reduction of CO <sub>2</sub> on Cu and Ag. <i>Accounts of Chemical Research</i> , 2022, 55, 484-494.	7.6	81
6	Mechanism and Kinetics of <i>n</i> -Butane Dehydrogenation to 1,3-Butadiene Catalyzed by Isolated Pt Sites Grafted onto -SiO <sub>2</sub> -OH Nests in Dealuminated Zeolite Beta. <i>ACS Catalysis</i> , 2022, 12, 3333-3345.	5.5	18
7	Highly selective and productive reduction of carbon dioxide to multicarbon products via in situ CO management using segmented tandem electrodes. <i>Nature Catalysis</i> , 2022, 5, 202-211.	16.1	120
8	Pathways for the Formation of C <sub>2+</sub> Products under Alkaline Conditions during the Electrochemical Reduction of CO <sub>2</sub> . <i>ACS Energy Letters</i> , 2022, 7, 1679-1686.	8.8	27
9	Continuum Modeling of Porous Electrodes for Electrochemical Synthesis. <i>Chemical Reviews</i> , 2022, 122, 11022-11084.	23.0	46
10	Assessing the stability of Pd-exchanged sites in zeolites with the aid of a high throughput quantum chemistry workflow. <i>Nature Communications</i> , 2022, 13, .	5.8	9
11	Siloxaluminato and Siloxygallate Complexes as Models for Framework and Partially Hydrolyzed Framework Sites in Zeolites and Zeotypes. <i>Chemistry - A European Journal</i> , 2021, 27, 307-315.	1.7	2
12	Challenges for density functional theory: calculation of CO adsorption on electrocatalytically relevant metals. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 9394-9406.	1.3	15
13	Mechanism and Kinetics of Light Alkane Dehydrogenation and Cracking over Isolated Ga Species in Ga/H-MFI. <i>ACS Catalysis</i> , 2021, 11, 2062-2075.	5.5	31
14	Mechanism and Kinetics of Acetone Conversion to Isobutene over Isolated Hf Sites Grafted to Silicalite-1 and SiO <sub>2</sub> . <i>Journal of the American Chemical Society</i> , 2021, 143, 8352-8366.	6.6	33
15	Critical Role of Thermal Fluctuations for CO Binding on Electrocatalytic Metal Surfaces. <i>Jacs Au</i> , 2021, 1, 1708-1718.	3.6	10
16	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	1.2	518
17	Few-Unit-Cell MFI Zeolite Synthesized using a Simple Di-quaternary Ammonium Structure-Directing Agent. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 19214-19221.	7.2	19
18	The Role of Roughening to Enhance Selectivity to C <sub>2+</sub> Products during CO <sub>2</sub> Electroreduction on Copper. <i>ACS Energy Letters</i> , 2021, 6, 3252-3260.	8.8	38

#	ARTICLE	IF	CITATIONS
19	Fewâ€Unitâ€™Cell MFI Zeolite Synthesized using a Simple Diâ€™quaternary Ammonium Structureâ€™Directing Agent. <i>Angewandte Chemie</i> , 2021, 133, 19363-19370.	1.6	8
20	Challenges for the theoretical description of the mechanism and kinetics of reactions catalyzed by zeolites. <i>Journal of Catalysis</i> , 2021, 404, 832-849.	3.1	6
21	Computational modeling predicts the stability of both Pd <sup>+</sup> and Pd <sup>2+</sup> ion-exchanged into H-CHA. <i>Journal of Materials Chemistry A</i> , 2021, 9, 2161-2174.	5.2	20
22	Kinetic modeling of nitrous oxide decomposition on Fe-ZSM-5 in the presence of nitric oxide based on parameters obtained from first-principles calculations. <i>Catalysis Science and Technology</i> , 2021, 11, 3539-3555.	2.1	3
23	Tailored catalyst microenvironments for CO <sub>2</sub> electroreduction to multicarbon products on copper using bilayer ionomer coatings. <i>Nature Energy</i> , 2021, 6, 1026-1034.	19.8	194
24	On the Nature of Field-Enhanced Water Dissociation in Bipolar Membranes. <i>Journal of Physical Chemistry C</i> , 2021, 125, 24974-24987.	1.5	17
25	Propane Dehydrogenation and Cracking over Zn/H-MFI Prepared by Solid-State Ion Exchange of ZnCl <sub>2</sub> . <i>ACS Catalysis</i> , 2021, 11, 14489-14506.	5.5	33
26	Propane Dehydrogenation Catalyzed by Isolated Pt Atoms in $\gamma$ -SiO <sub>2</sub> -OH Nests in Dealuminated Zeolite Beta. <i>Journal of the American Chemical Society</i> , 2021, 143, 21364-21378.	6.6	92
27	Electronic structure calculations permit identification of the driving forces behind frequency shifts in transition metal monocarbonyls. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 781-798.	1.3	21
28	Facing the Challenges of Borderline Oxidation State Assignments Using State-of-the-Art Computational Methods. <i>Inorganic Chemistry</i> , 2020, 59, 15410-15420.	1.9	27
29	The Role of Water in Vapor-fed Proton-Exchange-Membrane Electrolysis. <i>Journal of the Electrochemical Society</i> , 2020, 167, 104508.	1.3	34
30	Electrocatalytic CO <sub>2</sub> Reduction to Fuels: Progress and Opportunities. <i>Trends in Chemistry</i> , 2020, 2, 825-836.	4.4	104
31	Influence of surface Sn species and hydrogen interactions on the OH group formation over spherical silica-supported tin oxide catalysts. <i>Reaction Chemistry and Engineering</i> , 2020, 5, 1814-1823.	1.9	4
32	Ethanol Conversion to Butadiene over Isolated Zinc and Yttrium Sites Grafted onto Dealuminated Beta Zeolite. <i>Journal of the American Chemical Society</i> , 2020, 142, 14674-14687.	6.6	90
33	A Perspective on the Electrochemical Oxidation of Methane to Methanol in Membrane Electrode Assemblies. <i>ACS Energy Letters</i> , 2020, 5, 2954-2963.	8.8	45
34	A systematic analysis of Cu-based membrane-electrode assemblies for CO <sub>2</sub> reduction through multiphysics simulation. <i>Energy and Environmental Science</i> , 2020, 13, 3592-3606.	15.6	67
35	Scanning Nanobeam Diffraction and Energy Dispersive Spectroscopy Characterization of a Model Mn-Promoted Co/Al <sub>2</sub> O <sub>3</sub> Nanosphere Catalyst for Fischerâ€™Tropsch Synthesis. <i>ACS Catalysis</i> , 2020, 10, 12071-12079.	5.5	7
36	Understanding Multi-Ion Transport Mechanisms in Bipolar Membranes. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 52509-52526.	4.0	54

#	ARTICLE	IF	CITATIONS
37	Experimental and Computational Studies of Carbon–Carbon Bond Formation via Ketonization and Aldol Condensation over Site-Isolated Zirconium Catalysts. <i>ACS Catalysis</i> , 2020, 10, 4566-4579.	5.5	33
38	Effects of Surface Roughness on the Electrochemical Reduction of CO <sub>2</sub> over Cu. <i>ACS Energy Letters</i> , 2020, 5, 1206-1214.	8.8	172
39	Production of C <sub>2</sub> /C <sub>3</sub> Oxygenates from Planar Copper Nitride-Derived Mesoporous Copper via Electrochemical Reduction of CO <sub>2</sub> . <i>Chemistry of Materials</i> , 2020, 32, 3304-3311.	3.2	64
40	Heterogenized Pyridine-Substituted Cobalt(II) Phthalocyanine Yields Reduction of CO <sub>2</sub> by Tuning the Electron Affinity of the Co Center. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 5251-5258.	4.0	41
41	Impact of Pulsed Electrochemical Reduction of CO <sub>2</sub> on the Formation of C <sub>2+</sub> Products over Cu. <i>ACS Catalysis</i> , 2020, 10, 12403-12413.	5.5	83
42	Understanding cation effects in electrochemical CO <sub>2</sub> reduction. <i>Energy and Environmental Science</i> , 2019, 12, 3001-3014.	15.6	433
43	Factors and Dynamics of Cu Nanocrystal Reconstruction under CO <sub>2</sub> Reduction. <i>ACS Applied Energy Materials</i> , 2019, 2, 7744-7749.	2.5	56
44	Mechanism and Kinetics of Isobutene Formation from Ethanol and Acetone over Zn <sub>x</sub> Zr <sub>y</sub> O <sub>z</sub> . <i>ACS Catalysis</i> , 2019, 9, 10588-10604.	5.5	32
45	Synthesis of Biomass-Derived Ethers for Use as Fuels and Lubricants. <i>ChemSusChem</i> , 2019, 12, 2835-2858.	3.6	56
46	Zeolite-Catalyzed Isobutene Amination: Mechanism and Kinetics. <i>ACS Catalysis</i> , 2019, 9, 7012-7022.	5.5	19
47	Towards membrane-electrode assembly systems for CO <sub>2</sub> reduction: a modeling study. <i>Energy and Environmental Science</i> , 2019, 12, 1950-1968.	15.6	273
48	Response to –Impact of Zeolite Structure on Entropic–Enthalpic Contributions to Alkane Monomolecular Cracking: An IR Operando Study–. <i>Chemistry - A European Journal</i> , 2019, 25, 7225-7226.	1.7	1
49	Influence of Atomic Surface Structure on the Activity of Ag for the Electrochemical Reduction of CO <sub>2</sub> to CO. <i>ACS Catalysis</i> , 2019, 9, 4006-4014.	5.5	119
50	Explaining the Incorporation of Oxygen Derived from Solvent Water into the Oxygenated Products of CO Reduction over Cu. <i>Journal of the American Chemical Society</i> , 2019, 141, 4191-4193.	6.6	29
51	Propanol Amination over Supported Nickel Catalysts: Reaction Mechanism and Role of the Support. <i>ACS Catalysis</i> , 2019, 9, 2931-2939.	5.5	54
52	Mechanism and Kinetics of Propane Dehydrogenation and Cracking over Ga/H-MFI Prepared via Vapor-Phase Exchange of H-MFI with GaCl <sub>3</sub> . <i>Journal of the American Chemical Society</i> , 2019, 141, 1614-1627.	6.6	107
53	Challenges in Modeling Electrochemical Reaction Energetics with Polarizable Continuum Models. <i>ACS Catalysis</i> , 2019, 9, 920-931.	5.5	153
54	Understanding Brønsted-Acid Catalyzed Monomolecular Reactions of Alkanes in Zeolite Pores by Combining Insights from Experiment and Theory. <i>ChemPhysChem</i> , 2018, 19, 338-338.	1.0	0

#	ARTICLE	IF	CITATIONS
55	Impact of long-range electrostatic and dispersive interactions on theoretical predictions of adsorption and catalysis in zeolites. <i>Catalysis Today</i> , 2018, 312, 51-65.	2.2	35
56	Effects of Anion Identity and Concentration on Electrochemical Reduction of CO <sub>2</sub> . <i>ChemElectroChem</i> , 2018, 5, 1064-1072.	1.7	165
57	Is Subsurface Oxygen Necessary for the Electrochemical Reduction of CO <sub>2</sub> on Copper?. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 601-606.	2.1	118
58	Mechanism of CO <sub>2</sub> Reduction at Copper Surfaces: Pathways to C <sub>2</sub> Products. <i>ACS Catalysis</i> , 2018, 8, 1490-1499.	5.5	608
59	Atomistic Investigations of the Effects of Si/Al Ratio and Al Distribution on the Adsorption Selectivity of <i>n</i> -Alkanes in Brønsted-Acid Zeolites. <i>Journal of Physical Chemistry C</i> , 2018, 122, 9397-9410.	1.5	35
60	Understanding Brønsted-Acid Catalyzed Monomolecular Reactions of Alkanes in Zeolite Pores by Combining Insights from Experiment and Theory. <i>ChemPhysChem</i> , 2018, 19, 341-358.	1.0	21
61	Chapter 3. Understanding the Effects of Composition and Structure on the Oxygen Evolution Reaction (OER) Occurring on NiFeO <sub>x</sub> Catalysts. <i>RSC Energy and Environment Series</i> , 2018, , 79-116.	0.2	3
62	Reaction mechanism of the selective reduction of CO <sub>2</sub> to CO by a tetraaza [Co <sup>II</sup> N <sub>4</sub> H] <sup>2+</sup> complex in the presence of protons. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 24058-24064.	1.3	15
63	Characterization of Isolated Ga <sup>3+</sup> Cations in Ga/H-MFI Prepared by Vapor-Phase Exchange of H-MFI Zeolite with GaCl <sub>3</sub> . <i>ACS Catalysis</i> , 2018, 8, 6106-6126.	5.5	85
64	Continuous pervaporation-assisted furfural production catalyzed by CrCl <sub>3</sub> . <i>Green Chemistry</i> , 2018, 20, 2903-2912.	4.6	22
65	Standards and Protocols for Data Acquisition and Reporting for Studies of the Electrochemical Reduction of Carbon Dioxide. <i>ACS Catalysis</i> , 2018, 8, 6560-6570.	5.5	250
66	Direct Observation of the Local Reaction Environment during the Electrochemical Reduction of CO <sub>2</sub> . <i>Journal of the American Chemical Society</i> , 2018, 140, 7012-7020.	6.6	176
67	Computational Modeling of the Nature and Role of Ga Species for Light Alkane Dehydrogenation Catalyzed by Ga/H-MFI. <i>ACS Catalysis</i> , 2018, 8, 6146-6162.	5.5	86
68	Effect of Alcohol Structure on the Kinetics of Etherification and Dehydration over Tungstated Zirconia. <i>ChemSusChem</i> , 2018, 11, 3104-3111.	3.6	25
69	The mechanism and kinetics of methyl isobutyl ketone synthesis from acetone over ion-exchanged hydroxyapatite. <i>Journal of Catalysis</i> , 2018, 365, 174-183.	3.1	25
70	Nonempirical Meta-Generalized Gradient Approximations for Modeling Chemisorption at Metal Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3083-3090.	2.3	20
71	Modeling gas-diffusion electrodes for CO <sub>2</sub> reduction. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 16973-16984.	1.3	305
72	Theoretical Analysis of the Influence of Pore Geometry on Monomolecular Cracking and Dehydrogenation of <i>n</i> -Butane in Brønsted Acidic Zeolites. <i>ACS Catalysis</i> , 2017, 7, 2685-2697.	5.5	42

#	ARTICLE	IF	CITATIONS
73	Production of Biomass-Based Automotive Lubricants by Reductive Etherification. <i>ChemSusChem</i> , 2017, 10, 2527-2533.	3.6	31
74	Optimizing C-C Coupling on Oxide-Derived Copper Catalysts for Electrochemical CO <sub>2</sub> Reduction. <i>Journal of Physical Chemistry C</i> , 2017, 121, 14191-14203.	1.5	254
75	Artificial neural network based predictions of cetane number for furanic biofuel additives. <i>Fuel</i> , 2017, 206, 171-179.	3.4	60
76	Effects of Pore and Cage Topology on the Thermodynamics of <i>n</i> -Alkane Adsorption at Brønsted Protons in Zeolites at High Temperature. <i>Journal of Physical Chemistry C</i> , 2017, 121, 1618-1638.	1.5	17
77	Mechanistic insights into electrochemical reduction of CO <sub>2</sub> over Ag using density functional theory and transport models. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E8812-E8821.	3.3	219
78	Mechanism and kinetics of 1-dodecanol etherification over tungstated zirconia. <i>Journal of Catalysis</i> , 2017, 354, 13-23.	3.1	25
79	Nanoporous gold assemblies of calixarene-phosphine-capped colloids. <i>Chemical Communications</i> , 2017, 53, 10870-10873.	2.2	4
80	Integrated catalytic sequences for catalytic upgrading of bio-derived carboxylic acids to fuels, lubricants and chemical feedstocks. <i>Sustainable Energy and Fuels</i> , 2017, 1, 1805-1809.	2.5	20
81	Novel Strategies for the Production of Fuels, Lubricants, and Chemicals from Biomass. <i>Accounts of Chemical Research</i> , 2017, 50, 2589-2597.	7.6	159
82	Promoter Effects of Alkali Metal Cations on the Electrochemical Reduction of Carbon Dioxide. <i>Journal of the American Chemical Society</i> , 2017, 139, 11277-11287.	6.6	653
83	Electrochemical CO <sub>2</sub> Reduction over Compressively Strained CuAg Surface Alloys with Enhanced Multi-Carbon Oxygenate Selectivity. <i>Journal of the American Chemical Society</i> , 2017, 139, 15848-15857.	6.6	470
84	A DFT Investigation of the Mechanism of Propene Ammoxidation over $\delta$ -Bismuth Molybdate. <i>ACS Catalysis</i> , 2017, 7, 161-176.	5.5	26
85	Kinetics of hydrogenation and hydrogenolysis of 2,5-dimethylfuran over noble metals catalysts under mild conditions. <i>Applied Catalysis B: Environmental</i> , 2017, 202, 557-568.	10.8	41
86	Ga[OSi(O <sup>t</sup> Bu) <sub>3</sub> ] <sub>3</sub> ·THF, a thermolytic molecular precursor for high surface area gallium-containing silica materials of controlled dispersion and stoichiometry. <i>Dalton Transactions</i> , 2016, 45, 11025-11034.	1.6	18
87	From Sugars to Wheels: The Conversion of Ethanol to 1,3-Butadiene over Metal-Promoted Magnesia-Silicate Catalysts. <i>ChemSusChem</i> , 2016, 9, 1462-1472.	3.6	84
88	CO <sub>2</sub> Electroreduction with Enhanced Ethylene and Ethanol Selectivity by Nanostructuring Polycrystalline Copper. <i>ChemElectroChem</i> , 2016, 3, 1012-1019.	1.7	142
89	Theoretical Study of 4-(Hydroxymethyl)benzoic Acid Synthesis from Ethylene and 5-(Hydroxymethyl)furoic Acid Catalyzed by Sn-BEA. <i>ACS Catalysis</i> , 2016, 6, 5052-5061.	5.5	18
90	Identifying the Unique Properties of $\delta$ -Bi <sub>2</sub> Mo <sub>3</sub> O <sub>12</sub> for the Activation of Propene. <i>Journal of Physical Chemistry C</i> , 2016, 120, 29233-29247.	1.5	9

#	ARTICLE	IF	CITATIONS
91	Growth of encapsulating carbon on supported Pt nanoparticles studied by in situ TEM. <i>Journal of Catalysis</i> , 2016, 338, 295-304.	3.1	39
92	Effects of Lewis acidity of metal oxide promoters on the activity and selectivity of Co-based Fischer-Tropsch synthesis catalysts. <i>Journal of Catalysis</i> , 2016, 338, 250-264.	3.1	71
93	The mechanism and kinetics of propene ammoxidation over $\gamma$ -bismuth molybdate. <i>Journal of Catalysis</i> , 2016, 339, 228-241.	3.1	22
94	Thermodynamics of Anharmonic Systems: Uncoupled Mode Approximations for Molecules. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2861-2870.	2.3	38
95	Identification of Possible Pathways for C-C Bond Formation during Electrochemical Reduction of CO <sub>2</sub> : New Theoretical Insights from an Improved Electrochemical Model. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1471-1477.	2.1	479
96	Experimental and Computational Evidence of Highly Active Fe Impurity Sites on the Surface of Oxidized Au for the Electrocatalytic Oxidation of Water in Basic Media. <i>ChemElectroChem</i> , 2016, 3, 66-73.	1.7	44
97	Pervaporation-assisted catalytic conversion of xylose to furfural. <i>Green Chemistry</i> , 2016, 18, 4073-4085.	4.6	28
98	Effects of temperature and gas-liquid mass transfer on the operation of small electrochemical cells for the quantitative evaluation of CO <sub>2</sub> reduction electrocatalysts. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 26777-26785.	1.3	138
99	Production of Hydroxyl-rich Acids from Xylose and Glucose Using Sn-BEA Zeolite. <i>ChemistrySelect</i> , 2016, 1, 4167-4172.	0.7	27
100	Effects of Composition and Structure of Mg/Al Oxides on Their Activity and Selectivity for the Condensation of Methyl Ketones. <i>Industrial &amp; Engineering Chemistry Research</i> , 2016, 55, 10635-10644.	1.8	32
101	Propene Metathesis over Supported Tungsten Oxide Catalysts: A Study of Active Site Formation. <i>ACS Catalysis</i> , 2016, 6, 7728-7738.	5.5	60
102	Quantum Mechanical Screening of Single-Atom Bimetallic Alloys for the Selective Reduction of CO <sub>2</sub> to C <sub>1</sub> Hydrocarbons. <i>ACS Catalysis</i> , 2016, 6, 7769-7777.	5.5	190
103	Hydrolysis of Electrolyte Cations Enhances the Electrochemical Reduction of CO <sub>2</sub> over Ag and Cu. <i>Journal of the American Chemical Society</i> , 2016, 138, 13006-13012.	6.6	640
104	Operando Analyses of Solar Fuels Light Absorbers and Catalysts. <i>Electrochimica Acta</i> , 2016, 211, 711-719.	2.6	23
105	Delignification of miscanthus using ethylenediamine (EDA) with or without ammonia and subsequent enzymatic hydrolysis to sugars. <i>3 Biotech</i> , 2016, 6, 23.	1.1	11
106	Effects of Zeolite Structural Confinement on Adsorption Thermodynamics and Reaction Kinetics for Monomolecular Cracking and Dehydrogenation of <i>n</i> -Butane. <i>Journal of the American Chemical Society</i> , 2016, 138, 4739-4756.	6.6	72
107	A systematic study on Pt based, subnanometer-sized alloy cluster catalysts for alkane dehydrogenation: effects of intermetallic interaction. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 10906-10917.	1.3	29
108	Production of renewable lubricants via self-condensation of methyl ketones. <i>Green Chemistry</i> , 2016, 18, 3577-3581.	4.6	29

#	ARTICLE	IF	CITATIONS
109	The role of hydrogen during Ptâ€“Ga nanocatalyst formation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 3234-3243.	1.3	27
110	Ambient-Pressure XPS Study of a Niâ€“Fe Electrocatalyst for the Oxygen Evolution Reaction. <i>Journal of Physical Chemistry C</i> , 2016, 120, 2247-2253.	1.5	336
111	Mechanism and Kinetics of Ethanol Coupling to Butanol over Hydroxyapatite. <i>ACS Catalysis</i> , 2016, 6, 939-948.	5.5	139
112	Trace Levels of Copper in Carbon Materials Show Significant Electrochemical CO <sub>2</sub> Reduction Activity. <i>ACS Catalysis</i> , 2016, 6, 202-209.	5.5	143
113	Role of ZrO <sub>2</sub> in Promoting the Activity and Selectivity of Co-Based Fischerâ€“Tropsch Synthesis Catalysts. <i>ACS Catalysis</i> , 2016, 6, 100-114.	5.5	56
114	Design of an artificial photosynthetic system for production of alcohols in high concentration from CO <sub>2</sub> . <i>Energy and Environmental Science</i> , 2016, 9, 193-199.	15.6	47
115	Effects of catalyst crystal structure on the oxidation of propene to acrolein. <i>Catalysis Today</i> , 2016, 261, 146-153.	2.2	22
116	Non-Oxidative Dehydrogenation Pathways for the Conversion of C <sub>2</sub> -C <sub>4</sub> Alcohols to Carbonyl Compounds. <i>ChemSusChem</i> , 2015, 8, 3917-3917.	3.6	0
117	Upgrading Lignocellulosic Products to Dropâ€“In Biofuels via Dehydrogenative Crossâ€“Coupling and Hydrodeoxygenation Sequence. <i>ChemSusChem</i> , 2015, 8, 2609-2614.	3.6	31
118	Nonâ€“Oxidative Dehydrogenation Pathways for the Conversion of C <sub>2</sub> â€“C <sub>4</sub> Alcohols to Carbonyl Compounds. <i>ChemSusChem</i> , 2015, 8, 3959-3962.	3.6	11
119	Adsorption Thermodynamics and Intrinsic Activation Parameters for Monomolecular Cracking of <i>n</i> -Alkanes on Brønsted Acid Sites in Zeolites. <i>Journal of Physical Chemistry C</i> , 2015, 119, 10427-10438.	1.5	48
120	Novel pathways for fuels and lubricants from biomass optimized using life-cycle greenhouse gas assessment. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 7645-7649.	3.3	101
121	Investigations of element spatial correlation in Mn-promoted Co-based Fischerâ€“Tropsch synthesis catalysts. <i>Journal of Catalysis</i> , 2015, 328, 111-122.	3.1	29
122	Catalytic Upgrading of Biomassâ€“Derived Methyl Ketones to Liquid Transportation Fuel Precursors by an Organocatalytic Approach. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 4673-4677.	7.2	63
123	Selective oxidation and oxidative dehydrogenation of hydrocarbons on bismuth vanadium molybdenum oxide. <i>Journal of Catalysis</i> , 2015, 325, 87-100.	3.1	47
124	Pretreatment of <i>Miscanthus giganteus</i> with Lime and Oxidants for Biofuels. <i>Energy &amp; Fuels</i> , 2015, 29, 1743-1750.	2.5	8
125	Improved Force-Field Parameters for QM/MM Simulations of the Energies of Adsorption for Molecules in Zeolites and a Free Rotor Correction to the Rigid Rotor Harmonic Oscillator Model for Adsorption Enthalpies. <i>Journal of Physical Chemistry C</i> , 2015, 119, 1840-1850.	1.5	110
126	Synthesis of biomass-derived methylcyclopentane as a gasoline additive via aldol condensation/hydrodeoxygenation of 2,5-hexanedione. <i>Green Chemistry</i> , 2015, 17, 2393-2397.	4.6	64



#	ARTICLE	IF	CITATIONS
127	The Role of Metal Halides in Enhancing the Dehydration of Xylose to Furfural. <i>ChemCatChem</i> , 2015, 7, 479-489.	1.8	74
128	Identification of Highly Active Fe Sites in (Ni,Fe)OOH for Electrocatalytic Water Splitting. <i>Journal of the American Chemical Society</i> , 2015, 137, 1305-1313.	6.6	2,018
129	p-Type Transparent Conducting Oxide/n-Type Semiconductor Heterojunctions for Efficient and Stable Solar Water Oxidation. <i>Journal of the American Chemical Society</i> , 2015, 137, 9595-9603.	6.6	122
130	Role of Catalyst Preparation on the Electrocatalytic Activity of Ni <sub>x</sub> Fe <sub>x</sub> OOH for the Oxygen Evolution Reaction. <i>Journal of Physical Chemistry C</i> , 2015, 119, 18303-18316.	1.5	114
131	Effects of electrolyte, catalyst, and membrane composition and operating conditions on the performance of solar-driven electrochemical reduction of carbon dioxide. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 18924-18936.	1.3	312
132	SnCl <sub>4</sub> -catalyzed isomerization/dehydration of xylose and glucose to furanics in water. <i>Catalysis Science and Technology</i> , 2015, 5, 2839-2847.	2.1	89
133	Highly Selective Condensation of Biomass-Derived Methyl Ketones as a Source of Aviation Fuel. <i>ChemSusChem</i> , 2015, 8, 1726-1736.	3.6	105
134	Nitric-acid hydrolysis of <i>Miscanthus giganteus</i> to sugars fermented to bioethanol. <i>Biotechnology and Bioprocess Engineering</i> , 2015, 20, 304-314.	1.4	17
135	An Atomic-Scale View of the Nucleation and Growth of Graphene Islands on Pt Surfaces. <i>Journal of Physical Chemistry C</i> , 2015, 119, 7124-7129.	1.5	21
136	Effects of Fe Electrolyte Impurities on Ni(OH) <sub>2</sub> /NiOOH Structure and Oxygen Evolution Activity. <i>Journal of Physical Chemistry C</i> , 2015, 119, 7243-7254.	1.5	806
137	Tailoring Metal-Porphyrin-Like Active Sites on Graphene to Improve the Efficiency and Selectivity of Electrochemical CO <sub>2</sub> Reduction. <i>Journal of Physical Chemistry C</i> , 2015, 119, 21345-21352.	1.5	79
138	Thermodynamic and achievable efficiencies for solar-driven electrochemical reduction of carbon dioxide to transportation fuels. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, E6111-8.	3.3	103
139	Differential Electrochemical Mass Spectrometer Cell Design for Online Quantification of Products Produced during Electrochemical Reduction of CO <sub>2</sub> . <i>Analytical Chemistry</i> , 2015, 87, 8013-8020.	3.2	83
140	Wavefunction stability analysis without analytical electronic Hessians: application to orbital-optimised second-order Møller-Plesset theory and VV10-containing density functionals. <i>Molecular Physics</i> , 2015, 113, 1802-1808.	0.8	30
141	Electrochemical Study of the Energetics of the Oxygen Evolution Reaction at Nickel Iron (Oxy)Hydroxide Catalysts. <i>Journal of Physical Chemistry C</i> , 2015, 119, 19022-19029.	1.5	282
142	Ethane and propane dehydrogenation over PtIr/Mg(Al)O. <i>Applied Catalysis A: General</i> , 2015, 506, 25-32.	2.2	64
143	An Investigation into the Effects of Mn Promotion on the Activity and Selectivity of Co/SiO <sub>2</sub> for Fischer-Tropsch Synthesis: Evidence for Enhanced CO Adsorption and Dissociation. <i>ACS Catalysis</i> , 2015, 5, 5888-5903.	5.5	138
144	The Role of Hydroxyl Group Acidity on the Activity of Silica-Supported Secondary Amines for the Self-Condensation of n-Butanal. <i>ChemSusChem</i> , 2015, 8, 466-472.	3.6	30

#	ARTICLE	IF	CITATIONS
145	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	0.8	2,561
146	How to Chemically Tailor Metal-Porphyrin-Like Active Sites on Carbon Nanotubes and Graphene for Minimal Overpotential in the Electrochemical Oxygen Evolution and Oxygen Reduction Reactions. <i>Journal of Physical Chemistry C</i> , 2014, 118, 29482-29491.	1.5	36
147	A finite difference Davidson procedure to sidestep full <i>ab initio</i> hessian calculation: Application to characterization of stationary points and transition state searches. <i>Journal of Chemical Physics</i> , 2014, 140, 164115.	1.2	25
148	Syntheses of Biodiesel Precursors: Sulfonic Acid Catalysts for Condensation of Biomass-Derived Platform Molecules. <i>ChemSusChem</i> , 2014, 7, 945-945.	3.6	0
149	Selective Hydrogenation of Furan-Containing Condensation Products as a Source of Biomass-Derived Diesel Additives. <i>ChemSusChem</i> , 2014, 7, 2796-2800.	3.6	40
150	Effects of composition and metal particle size on ethane dehydrogenation over Pt <sub>x</sub> Sn <sub>100-x</sub> /Mg(Al)O (70 ≤ x ≤ 100). <i>Journal of Catalysis</i> , 2014, 311, 161-168.	3.1	109
151	n-Butane dehydrogenation over Pt/Mg(In)(Al)O. <i>Applied Catalysis A: General</i> , 2014, 470, 208-214.	2.2	38
152	Biomass conversion to diesel via the etherification of furanyl alcohols catalyzed by Amberlyst-15. <i>Journal of Catalysis</i> , 2014, 313, 70-79.	3.1	101
153	Hydrogenation of butanal over silica-supported Shvo's catalyst and its use for the gas-phase conversion of propene to butanol via tandem hydroformylation and hydrogenation. <i>Journal of Catalysis</i> , 2014, 311, 52-58.	3.1	20
154	Tailoring the Cooperative Acid-Base Effects in Silica-Supported Amine Catalysts: Applications in the Continuous Gas-Phase Self-Condensation of n-Butanal. <i>ChemCatChem</i> , 2014, 6, 1283-1290.	1.8	28
155	Syntheses of Biodiesel Precursors: Sulfonic Acid Catalysts for Condensation of Biomass-Derived Platform Molecules. <i>ChemSusChem</i> , 2014, 7, 1078-1085.	3.6	58
156	Propene Oligomerization using Alkali Metal- and Nickel-Exchanged Mesoporous Aluminosilicate Catalysts. <i>ACS Catalysis</i> , 2014, 4, 337-343.	5.5	48
157	Selective Propene Oligomerization with Nickel(II)-Based Metal-Organic Frameworks. <i>ACS Catalysis</i> , 2014, 4, 717-721.	5.5	87
158	Reaction Dynamics of Zeolite-Catalyzed Alkene Methylation by Methanol. <i>Journal of Physical Chemistry C</i> , 2014, 118, 21409-21419.	1.5	29
159	Two-Step Delignification of Miscanthus To Enhance Enzymatic Hydrolysis: Aqueous Ammonia Followed by Sodium Hydroxide and Oxidants. <i>Energy &amp; Fuels</i> , 2014, 28, 542-548.	2.5	10
160	Functionalized Graphene as a Gatekeeper for Chiral Molecules: An Alternative Concept for Chiral Separation. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 9957-9960.	7.2	44
161	Experimental and Theoretical Study of n-Butanal Self-Condensation over Ti Species Supported on Silica. <i>ACS Catalysis</i> , 2014, 4, 2908-2916.	5.5	34
162	Discovering Ce-rich oxygen evolution catalysts, from high throughput screening to water electrolysis. <i>Energy and Environmental Science</i> , 2014, 7, 682-688.	15.6	165

#	ARTICLE	IF	CITATIONS
163	Computational Study of <i>p</i> -Xylene Synthesis from Ethylene and 2,5-Dimethylfuran Catalyzed by H-BEA. <i>Journal of Physical Chemistry C</i> , 2014, 118, 22090-22095.	1.5	64
164	Analysis of the Reaction Mechanism and Catalytic Activity of Metal-Substituted Beta Zeolite for the Isomerization of Glucose to Fructose. <i>ACS Catalysis</i> , 2014, 4, 1537-1545.	5.5	148
165	Synthesis and Characterization of Supported Cobalt–Manganese Nanoparticles as Model Catalysts for Fischer–Tropsch Synthesis. <i>ChemCatChem</i> , 2014, 6, 2881-2888.	1.8	33
166	Single iron sites for catalytic, nonoxidative conversion of methane. <i>Science China Chemistry</i> , 2014, 57, 923-923.	4.2	6
167	Band-Gap Energy as a Descriptor of Catalytic Activity for Propene Oxidation over Mixed Metal Oxide Catalysts. <i>Journal of the American Chemical Society</i> , 2014, 136, 13684-13697.	6.6	120
168	Preparation and Characterization of High-Surface-Area Bi <sub>3</sub> VMoO <sub>4</sub> Catalysts. <i>Langmuir</i> , 2014, 30, 873-880.	1.6	17
169	Pretreatment of <i>Miscanthus</i> – <i>giganteus</i> using aqueous ammonia with hydrogen peroxide to increase enzymatic hydrolysis to sugars. <i>Journal of Chemical Technology and Biotechnology</i> , 2014, 89, 698-706.	1.6	28
170	An Investigation of Thin-Film Ni–Fe Oxide Catalysts for the Electrochemical Evolution of Oxygen. <i>Journal of the American Chemical Society</i> , 2013, 135, 12329-12337.	6.6	2,132
171	Water oxidation catalysis via immobilization of the dimanganese complex [Mn <sub>2</sub> ( <sup>1/4</sup> -O)Cl( <sup>1/4</sup> -O <sub>2</sub> CCH <sub>3</sub> )(bpy) <sub>2</sub> (H <sub>2</sub> O)](NO <sub>3</sub> ) <sub>2</sub> onto silica. <i>Dalton Transactions</i> , 2013, 42, 12238.	1.6	12
172	The Effect of Noncatalytic Cations on the Activity and Selectivity of Nickel–Exchanged X–Zeolites for Propene Oligomerization. <i>ChemCatChem</i> , 2013, 5, 3139-3147.	1.8	21
173	Theoretical Investigation of the Activity of Cobalt Oxides for the Electrochemical Oxidation of Water. <i>Journal of the American Chemical Society</i> , 2013, 135, 13521-13530.	6.6	1,093
174	Aqueous-ammonia delignification of miscanthus followed by enzymatic hydrolysis to sugars. <i>Bioresource Technology</i> , 2013, 135, 23-29.	4.8	44
175	The Influence of Functionals on Density Functional Theory Calculations of the Properties of Reducible Transition Metal Oxide Catalysts. <i>Journal of Physical Chemistry C</i> , 2013, 117, 25562-25578.	1.5	47
176	On the chemical state of Co oxide electrocatalysts during alkaline water splitting. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 17460.	1.3	89
177	DFT+U Investigation of Propene Oxidation over Bismuth Molybdate: Active Sites, Reaction Intermediates, and the Role of Bismuth. <i>Journal of Physical Chemistry C</i> , 2013, 117, 7123-7137.	1.5	70
178	Preferential Interactions between Lithium Chloride and Glucan Chains in <i>N,N</i> -Dimethylacetamide Drive Cellulose Dissolution. <i>Journal of Physical Chemistry B</i> , 2013, 117, 3280-3286.	1.2	29
179	Insights into the Kinetics of Cracking and Dehydrogenation Reactions of Light Alkanes in H-MFI. <i>Journal of Physical Chemistry C</i> , 2013, 117, 12600-12611.	1.5	59
180	The kinetics of selective oxidation of propene on bismuth vanadium molybdenum oxide catalysts. <i>Journal of Catalysis</i> , 2013, 308, 25-36.	3.1	64

#	ARTICLE	IF	CITATIONS
181	In Situ Formation of Wilkinson-Type Hydroformylation Catalysts: Insights into the Structure, Stability, and Kinetics of Triphenylphosphine- and Xantphos-Modified Rh/SiO <sub>2</sub> . ACS Catalysis, 2013, 3, 348-357.	5.5	36
182	Subnanometer-sized Pt/Sn alloy cluster catalysts for the dehydrogenation of linear alkanes. Physical Chemistry Chemical Physics, 2013, 15, 20727.	1.3	75
183	Effects of Si/Al Ratio on the Distribution of Framework Al and on the Rates of Alkane Monomolecular Cracking and Dehydrogenation in H-MFI. Journal of the American Chemical Society, 2013, 135, 19193-19207.	6.6	187
184	Entropy of cellulose dissolution in water and in the ionic liquid 1-butyl-3-methylimidazolium chloride. Physical Chemistry Chemical Physics, 2012, 14, 8425.	1.3	46
185	Accurate Prediction of Hydrocarbon Interactions with Zeolites Utilizing Improved Exchange-Correlation Functionals and QM/MM Methods: Benchmark Calculations of Adsorption Enthalpies and Application to Ethene Methylation by Methanol. Journal of Physical Chemistry C, 2012, 116, 15406-15414.	1.5	47
186	Surfactant-free preparation of supported cubic platinum nanoparticles. Chemical Communications, 2012, 48, 1854.	2.2	45
187	The kinetics of Brønsted acid-catalyzed hydrolysis of hemicellulose dissolved in 1-ethyl-3-methylimidazolium chloride. RSC Advances, 2012, 2, 10028.	1.7	46
188	Automated Transition State Searches without Evaluating the Hessian. Journal of Chemical Theory and Computation, 2012, 8, 5166-5174.	2.3	68
189	Propene oligomerization over Ni-exchanged Na-X zeolites. Journal of Catalysis, 2012, 296, 156-164.	3.1	71
190	Importance of Correlation in Determining Electrocatalytic Oxygen Evolution Activity on Cobalt Oxides. Journal of Physical Chemistry C, 2012, 116, 21077-21082.	1.5	305
191	Factors Influencing the Activity, Selectivity, and Stability of Rh-Based Supported Ionic Liquid Phase (SILP) Catalysts for Hydroformylation of Propene. ACS Catalysis, 2012, 2, 487-493.	5.5	52
192	Size and Composition Control of Pt-In Nanoparticles Prepared by Seed-Mediated Growth Using Bimetallic Seeds. Langmuir, 2012, 28, 3345-3349.	1.6	12
193	A Theoretical Study of Methanol Oxidation Catalyzed by Isolated Vanadia Clusters Supported on the (101) Surface of Anatase. Journal of Physical Chemistry C, 2012, 116, 18728-18735.	1.5	22
194	Ab Initio Simulations Reveal that Reaction Dynamics Strongly Affect Product Selectivity for the Cracking of Alkanes over H-MFI. Journal of the American Chemical Society, 2012, 134, 19468-19476.	6.6	66
195	Experimental and theoretical investigation of the oxidative carbonylation of toluene to toluic acid catalyzed by palladium(II) in the presence of vanadium and molecular oxygen. Journal of Molecular Catalysis A, 2012, 361-362, 91-97.	4.8	5
196	The kinetics of gas-phase propene hydroformylation over a supported ionic liquid-phase (SILP) rhodium catalyst. Journal of Catalysis, 2012, 292, 166-172.	3.1	29
197	Restricted active space spin-flip configuration interaction: Theory and examples for multiple spin flips with odd numbers of electrons. Journal of Chemical Physics, 2012, 137, 164110.	1.2	69
198	Delignification of Miscanthus by Extraction. Separation Science and Technology, 2012, 47, 370-376.	1.3	9

#	ARTICLE	IF	CITATIONS
199	In Situ Raman Study of Nickel Oxide and Gold-Supported Nickel Oxide Catalysts for the Electrochemical Evolution of Oxygen. <i>Journal of Physical Chemistry C</i> , 2012, 116, 8394-8400.	1.5	609
200	Etherification and reductive etherification of 5-(hydroxymethyl)furfural: 5-(alkoxymethyl)furfurals and 2,5-bis(alkoxymethyl)furans as potential bio-diesel candidates. <i>Green Chemistry</i> , 2012, 14, 1626.	4.6	347
201	Investigation of the structure and activity of VO <sub>x</sub> /CeO <sub>2</sub> /SiO <sub>2</sub> catalysts for methanol oxidation to formaldehyde. <i>Journal of Catalysis</i> , 2012, 285, 160-167.	3.1	34
202	High-resolution in situ and ex situ TEM studies on graphene formation and growth on Pt nanoparticles. <i>Journal of Catalysis</i> , 2012, 286, 22-29.	3.1	97
203	Effects of Brønsted-acid site proximity on the oligomerization of propene in H-MFI. <i>Journal of Catalysis</i> , 2012, 288, 65-73.	3.1	91
204	Effects of Mn promotion on the activity and selectivity of Co/SiO <sub>2</sub> for Fischer-Tropsch Synthesis. <i>Journal of Catalysis</i> , 2012, 288, 104-114.	3.1	143
205	Effects of reaction conditions on the acid-catalyzed hydrolysis of miscanthus dissolved in an ionic liquid. <i>Green Chemistry</i> , 2011, 13, 1467.	4.6	32
206	Calibration of the DFT/GGA+U Method for Determination of Reduction Energies for Transition and Rare Earth Metal Oxides of Ti, V, Mo, and Ce. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2218-2223.	2.3	215
207	Efficient exploration of reaction paths via a freezing string method. <i>Journal of Chemical Physics</i> , 2011, 135, 224108.	1.2	154
208	Incorporating Linear Synchronous Transit Interpolation into the Growing String Method: Algorithm and Applications. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 4019-4025.	2.3	37
209	Synthesis of Different CeO <sub>2</sub> Structures on Mesoporous Silica and Characterization of Their Reduction Properties. <i>Journal of Physical Chemistry C</i> , 2011, 115, 4114-4126.	1.5	56
210	Selection and Validation of Charge and Lennard-Jones Parameters for QM/MM Simulations of Hydrocarbon Interactions with Zeolites. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1695-1703.	2.3	67
211	Effects of the Synthesis Parameters on the Size and Composition of Pt-Sn Nanoparticles Prepared by the Polyalcohol Reduction Method. <i>Journal of Physical Chemistry C</i> , 2011, 115, 19084-19090.	1.5	27
212	Enhanced Activity of Gold-Supported Cobalt Oxide for the Electrochemical Evolution of Oxygen. <i>Journal of the American Chemical Society</i> , 2011, 133, 5587-5593.	6.6	1,264
213	Quantum Mechanical Modeling of Catalytic Processes. <i>Annual Review of Chemical and Biomolecular Engineering</i> , 2011, 2, 453-477.	3.3	68
214	Thermodynamics of Cellulose Solvation in Water and the Ionic Liquid 1-Butyl-3-Methylimidazolium Chloride. <i>Journal of Physical Chemistry B</i> , 2011, 115, 13433-13440.	1.2	86
215	Novel Pt/Mg(In)(Al)O catalysts for ethane and propane dehydrogenation. <i>Journal of Catalysis</i> , 2011, 282, 165-174.	3.1	206
216	Investigation of the structure and activity of VO <sub>x</sub> /ZrO <sub>2</sub> /SiO <sub>2</sub> catalysts for methanol oxidation to formaldehyde. <i>Journal of Catalysis</i> , 2011, 281, 222-230.	3.1	26

#	ARTICLE	IF	CITATIONS
217	Gas-Phase Hydroformylation of Propene over Silica-Supported PPh <sub>3</sub> -Modified Rhodium Catalysts. <i>Topics in Catalysis</i> , 2011, 54, 299-307.	1.3	19
218	A Study of the Acid-Catalyzed Hydrolysis of Cellulose Dissolved in Ionic Liquids and the Factors Influencing the Dehydration of Glucose and the Formation of Humins. <i>ChemSusChem</i> , 2011, 4, 1166-1173.	3.6	232
219	Comparison of Cobalt-based Nanoparticles as Electrocatalysts for Water Oxidation. <i>ChemSusChem</i> , 2011, 4, 1566-1569.	3.6	209
220	Recovery of glucose from an aqueous ionic liquid by adsorption onto a zeolite-based solid. <i>Chemical Engineering Journal</i> , 2011, 172, 184-190.	6.6	30
221	A Study of Oxygen Vacancy Formation and Annihilation in Submonolayer Coverages of TiO <sub>2</sub> Dispersed on MCM-48. <i>Journal of Physical Chemistry C</i> , 2010, 114, 16937-16945.	1.5	136
222	An experimental and theoretical investigation of the structure and reactivity of bilayered VO <sub>x</sub> /TiO <sub>x</sub> /SiO <sub>2</sub> catalysts for methanol oxidation. <i>Journal of Catalysis</i> , 2010, 270, 163-171.	3.1	37
223	Effect of zeolite framework type and Si/Al ratio on dimethoxymethane carbonylation. <i>Journal of Catalysis</i> , 2010, 270, 185-195.	3.1	52
224	Ethane dehydrogenation on Pt/Mg(Al)O and PtSn/Mg(Al)O catalysts. <i>Journal of Catalysis</i> , 2010, 271, 209-219.	3.1	199
225	An investigation into the mechanism and kinetics of dimethoxymethane carbonylation over FAU and MFI zeolites. <i>Journal of Catalysis</i> , 2010, 274, 150-162.	3.1	33
226	Catalyst performance of novel Pt/Mg(Ga)(Al)O catalysts for alkane dehydrogenation. <i>Journal of Catalysis</i> , 2010, 274, 200-206.	3.1	184
227	Synthesis and characterization of a new catalyst Pt/Mg(Ga)(Al)O for alkane dehydrogenation. <i>Journal of Catalysis</i> , 2010, 274, 192-199.	3.1	97
228	Effects of support composition and pretreatment on the activity and selectivity of carbon-supported PdCu <sub>n</sub> Cl <sub>x</sub> catalysts for the synthesis of diethyl carbonate. <i>Journal of Catalysis</i> , 2010, 276, 215-228.	3.1	26
229	Identification of Hydroperoxy Species as Reaction Intermediates in the Electrochemical Evolution of Oxygen on Gold. <i>ChemPhysChem</i> , 2010, 11, 1854-1857.	1.0	120
230	One-pot synthesis of alcohols from olefins catalyzed by rhodium and ruthenium complexes. <i>Applied Catalysis A: General</i> , 2010, 374, 201-212.	2.2	20
231	Reactor simulation of benzene ethylation and ethane dehydrogenation catalyzed by ZSM-5: A multiscale approach. <i>Chemical Engineering Science</i> , 2010, 65, 2472-2480.	1.9	33
232	A strategy for obtaining a more accurate transition state estimate using the growing string method. <i>Chemical Physics Letters</i> , 2010, 484, 392-398.	1.2	20
233	Theoretical Study of Zeolite-Catalyzed Dimethoxymethane Carbonylation to Methyl Methoxyacetate. <i>Journal of Physical Chemistry C</i> , 2010, 114, 17753-17760.	1.5	26
234	A two-step approach for the catalytic conversion of glucose to 2,5-dimethylfuran in ionic liquids. <i>Green Chemistry</i> , 2010, 12, 1253.	4.6	392

#	ARTICLE	IF	CITATIONS
235	Theoretical Simulation of n-Alkane Cracking on Zeolites. <i>Journal of Physical Chemistry C</i> , 2010, 114, 10229-10239.	1.5	73
236	Viscosities of the Mixtures of 1-Ethyl-3-Methylimidazolium Chloride with Water, Acetonitrile and Glucose: A Molecular Dynamics Simulation and Experimental Study. <i>Journal of Physical Chemistry B</i> , 2010, 114, 5790-5794.	1.2	52
237	Weak Interligand Interactions with Major Structural Consequences in Rh(CO) <sub>2</sub> (CF <sub>3</sub> COO) <sub>3</sub> . <i>Organometallics</i> , 2010, 29, 1144-1149.	1.1	2
238	Quantum Chemical Modeling of Benzene Ethylation over H-ZSM-5 Approaching Chemical Accuracy: A Hybrid MP2:DFT Study. <i>Journal of the American Chemical Society</i> , 2010, 132, 11525-11538.	6.6	144
239	Electron Donation in the Water–Water Hydrogen Bond. <i>Chemistry - A European Journal</i> , 2009, 15, 851-855.	1.7	135
240	Vapor–Phase Carbonylation of Dimethoxymethane over H <sub>2</sub> Faujasite. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 4813-4815.	7.2	29
241	Oxidative carbonylation of benzotrifluoride to form trifluoromethylbenzoic acid. <i>Journal of Molecular Catalysis A</i> , 2009, 302, 59-67.	4.8	11
242	Preparation of benzoyl fluoride from benzotrifluoride catalyzed by niobium oxide. <i>Applied Catalysis A: General</i> , 2009, 360, 33-37.	2.2	8
243	An investigation of carbon-supported CuCl <sub>2</sub> /PdCl <sub>2</sub> catalysts for diethyl carbonate synthesis. <i>Applied Catalysis A: General</i> , 2009, 366, 71-83.	2.2	46
244	The role of lattice oxygen in the oxidative dehydrogenation of ethane on alumina-supported vanadium oxide. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 6119.	1.3	32
245	Role of C–H Bond Strength in the Rate and Selectivity of Oxidative Dehydrogenation of Alkanes. <i>Journal of Physical Chemistry C</i> , 2009, 113, 12380-12386.	1.5	37
246	Effects of Ligand Composition on the Oxidative Carbonylation of Toluene to Toluic Acid Catalyzed by Rh(III) Complexes. <i>Journal of the American Chemical Society</i> , 2009, 131, 11098-11105.	6.6	23
247	Are Spin-Forbidden Crossings a Bottleneck in Methanol Oxidation?. <i>Journal of Physical Chemistry C</i> , 2009, 113, 19361-19364.	1.5	26
248	Are pressure fluctuation-based equilibrium methods really worse than nonequilibrium methods for calculating viscosities?. <i>Journal of Chemical Physics</i> , 2009, 131, 246101.	1.2	105
249	Transition state-finding strategies for use with the growing string method. <i>Journal of Chemical Physics</i> , 2009, 130, 244108.	1.2	49
250	Size-Dependent Activity of Co <sub>3</sub> O <sub>4</sub> Nanoparticle Anodes for Alkaline Water Electrolysis. <i>Journal of Physical Chemistry C</i> , 2009, 113, 15068-15072.	1.5	496
251	Spectroscopic investigation of the species involved in the rhodium-catalyzed oxidative carbonylation of toluene to toluic acid. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 9903.	1.3	13
252	Mechanism and Site Requirements for Ethanol Oxidation on Vanadium Oxide Domains. <i>Journal of Physical Chemistry C</i> , 2009, 113, 2830-2836.	1.5	104

#	ARTICLE	IF	CITATIONS
253	An Investigation of the Reduction and Reoxidation of Isolated Vanadate Sites Supported on MCM-48. <i>Catalysis Letters</i> , 2008, 122, 1-8.	1.4	8
254	Recent advances in catalysis—selected papers from APCAT 4 (Singapore, 6–8 December 2006). <i>Catalysis Today</i> , 2008, 131, 1.	2.2	5
255	Synthesis of precursors to ethylene glycol from formaldehyde and methyl formate catalyzed by heteropoly acids. <i>Journal of Molecular Catalysis A</i> , 2008, 288, 87-96.	4.8	77
256	Watching catalysts at work. <i>Nature</i> , 2008, 456, 185-186.	13.7	15
257	The mechanism of dimethyl carbonate synthesis on Cu-exchanged zeolite Y. <i>Journal of Catalysis</i> , 2008, 255, 153-161.	3.1	92
258	A Theoretical Investigation of Dimethyl Carbonate Synthesis on Cu <sup>2+</sup> /Y Zeolite. <i>Journal of Physical Chemistry C</i> , 2008, 112, 5043-5047.	1.5	53
259	Mechanistic Studies of the Hydroamination of Norbornene with Electrophilic Platinum Complexes: The Role of Proton Transfer. <i>Journal of the American Chemical Society</i> , 2008, 130, 16562-16571.	6.6	106
260	Analysis of charge transfer effects in molecular complexes based on absolutely localized molecular orbitals. <i>Journal of Chemical Physics</i> , 2008, 128, 184112.	1.2	188
261	Mechanistic Studies of Methanol Oxidation to Formaldehyde on Isolated Vanadate Sites Supported on High Surface Area Zirconia. <i>Journal of Physical Chemistry C</i> , 2008, 112, 6404-6412.	1.5	32
262	Theoretical Analysis of the Mechanism for the Oxidative Carbonylation of Toluene to <i>p</i> -Toluic Acid by Rhodium Complexes. <i>Journal of Physical Chemistry C</i> , 2008, 112, 2129-2136.	1.5	16
263	A Theoretical Investigation of the Selective Oxidation of Methanol to Formaldehyde on Isolated Vanadate Species Supported on Titania. <i>Journal of Physical Chemistry C</i> , 2008, 112, 13204-13214.	1.5	70
264	Theoretical Investigation of Benzene Alkylation with Ethene over H-ZSM-5. <i>Journal of Physical Chemistry C</i> , 2008, 112, 15402-15411.	1.5	78
265	Development and application of a hybrid method involving interpolation and <i>ab initio</i> calculations for the determination of transition states. <i>Journal of Chemical Physics</i> , 2008, 129, 174109.	1.2	41
266	Mechanistic Study of Iron(III) [Tetrakis(pentafluorophenyl)Porphyrin Triflate (F2OTPP)Fe(OTf)] Catalyzed Cyclooctene Epoxidation by Hydrogen Peroxide. <i>Inorganic Chemistry</i> , 2007, 46, 2278-2285.	1.9	41
267	Theoretical Study of Solvent Effects on the Thermodynamics of Iron(III) [Tetrakis(pentafluorophenyl)]porphyrin Chloride Dissociation. <i>Journal of Physical Chemistry B</i> , 2007, 111, 10992-10998.	1.2	10
268	Density Functional Theory Study of CO Adsorption on Cu(I)-ZSM-5. <i>Journal of Physical Chemistry C</i> , 2007, 111, 13442-13451.	1.5	20
269	A Reaction Mechanism for the Nitrous Oxide Decomposition on Binuclear Oxygen Bridged Iron Sites in Fe-ZSM-5. <i>Journal of Physical Chemistry C</i> , 2007, 111, 2092-2101.	1.5	80
270	A Theoretical Investigation of the Selective Oxidation of Methanol to Formaldehyde on Isolated Vanadate Species Supported on Silica. <i>Journal of Physical Chemistry C</i> , 2007, 111, 14753-14761.	1.5	74



#	ARTICLE	IF	CITATIONS
271	Mechanistic Studies of Methanol Oxidation to Formaldehyde on Isolated Vanadate Sites Supported on High Surface Area Anatase. <i>Journal of Physical Chemistry C</i> , 2007, 111, 14530-14540.	1.5	50
272	DFT Studies of the Structure and Vibrational Spectra of Isolated Molybdena Species Supported on Silica. <i>Journal of Physical Chemistry C</i> , 2007, 111, 1291-1298.	1.5	82
273	Mechanistic Studies of Methanol Oxidation to Formaldehyde on Isolated Vanadate Sites Supported on MCM-48. <i>Journal of Physical Chemistry C</i> , 2007, 111, 420-430.	1.5	67
274	Unravelling the Origin of Intermolecular Interactions Using Absolutely Localized Molecular Orbitals. <i>Journal of Physical Chemistry A</i> , 2007, 111, 8753-8765.	1.1	508
275	Effects of porphyrin composition on the activity and selectivity of the iron(III) porphyrin catalysts for the epoxidation of cyclooctene by hydrogen peroxide. <i>Journal of Molecular Catalysis A</i> , 2007, 272, 108-117.	4.8	35
276	Mechanistic insights into iron porphyrin-catalyzed olefin epoxidation by hydrogen peroxide: Factors controlling activity and selectivity. <i>Journal of Molecular Catalysis A</i> , 2007, 275, 54-62.	4.8	92
277	Oxidative carbonylation of toluene to p-toluic acid catalyzed by rhodium in the presence of vanadium and oxygen. <i>Journal of Molecular Catalysis A</i> , 2007, 276, 8-16.	4.8	21
278	An efficient self-consistent field method for large systems of weakly interacting components. <i>Journal of Chemical Physics</i> , 2006, 124, 204105.	1.2	179
279	Nitrous Oxide Decomposition over Fe-ZSM-5 in the Presence of Nitric Oxide: A Comprehensive DFT Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 17096-17114.	1.2	77
280	Density Functional Theory Analysis of the Reaction Pathway for Methane Oxidation to Acetic Acid Catalyzed by Pd <sup>2+</sup> in Sulfuric Acid. <i>Journal of the American Chemical Society</i> , 2006, 128, 4650-4657.	6.6	40
281	Stoichiometric and Catalytic Arene Activations by Platinum Complexes Containing Bidentate Monoanionic Nitrogen-Based Ligands. <i>Organometallics</i> , 2006, 25, 1801-1811.	1.1	71
282	Characterization of Cu-ZSM-5 Prepared by Solid-State Ion Exchange of H-ZSM-5 with CuCl. <i>Chemistry of Materials</i> , 2006, 18, 2347-2356.	3.2	55
283	Nature, Density, and Catalytic Role of Exposed Species on Dispersed VO <sub>x</sub> /CrO <sub>x</sub> /Al <sub>2</sub> O <sub>3</sub> Catalysts. <i>Journal of Physical Chemistry B</i> , 2006, 110, 2732-2739.	1.2	16
284	An In Situ Al K-Edge XAS Investigation of the Local Environment of H <sup>+</sup> - and Cu <sup>+</sup> -Exchanged USY and ZSM-5 Zeolites. <i>Journal of Physical Chemistry B</i> , 2006, 110, 11665-11676.	1.2	43
285	Stoichiometric and Catalytic Reactions Involving Si-H Bond Activations by Rh and Ir Complexes Containing a Pyridylindolide Ligand. <i>Organometallics</i> , 2006, 25, 4471-4482.	1.1	59
286	The Local Environment of Cu <sup>+</sup> in Cu <sup>+</sup> -Y Zeolite and Its Relationship to the Synthesis of Dimethyl Carbonate. <i>Journal of Physical Chemistry B</i> , 2006, 110, 11654-11664.	1.2	92
287	Effects of Methanol on the Thermodynamics of Iron(III) [Tetrakis(pentafluorophenyl)]porphyrin Chloride Dissociation and the Creation of Catalytically Active Species for the Epoxidation of Cyclooctene. <i>Inorganic Chemistry</i> , 2006, 45, 5591-5599.	1.9	26
288	Influence of Solvent Composition on the Kinetics of Cyclooctene Epoxidation by Hydrogen Peroxide Catalyzed by Iron(III) [tetrakis(pentafluorophenyl)] Porphyrin Chloride [(F <sub>2</sub> OTPP)FeCl]. <i>Inorganic Chemistry</i> , 2006, 45, 2758-2766.	1.9	28

#	ARTICLE	IF	CITATIONS
289	Study of the Elementary Processes Involved in the Selective Oxidation of Methane over MoO <sub>x</sub> /SiO <sub>2</sub> . Journal of Physical Chemistry B, 2006, 110, 2700-2709.	1.2	47
290	Efficient evaluation of the error vector in the direct inversion in the iterative subspace scheme. Chemical Physics Letters, 2006, 418, 359-360.	1.2	0
291	Pt-catalyzed oxidative carbonylation of methane to acetic acid in sulfuric acid. Journal of Molecular Catalysis A, 2006, 259, 296-301.	4.8	24
292	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	1.3	2,597
293	The influence of substrate composition on the kinetics of olefin epoxidation by hydrogen peroxide catalyzed by iron(III) [tetrakis(pentafluorophenyl)] porphyrin. Journal of Molecular Catalysis A, 2006, 258, 231-235.	4.8	25
294	Methane oxidation to acetic acid catalyzed by Pd <sup>2+</sup> cations in the presence of oxygen. Journal of Catalysis, 2006, 237, 111-117.	3.1	28
295	An investigation of the factors influencing the activity of Cu/Ce <sub>x</sub> Zr <sub>1-x</sub> O <sub>2</sub> for methanol synthesis via CO hydrogenation. Journal of Catalysis, 2006, 241, 276-286.	3.1	71
296	Effect of dopants on the activity of Cu/M <sub>0.3</sub> Zr <sub>0.7</sub> O <sub>2</sub> (M = Ce, Mn, and Pr) for CO hydrogenation to methanol. Journal of Catalysis, 2006, 244, 43-51.	3.1	35
297	Synthesis of dimethyl carbonate and dimethoxy methane over Cu-ZSM-5. Journal of Catalysis, 2006, 244, 219-229.	3.1	93
298	Quantum mechanical single molecule partition function from path integral Monte Carlo simulations. Journal of Chemical Physics, 2006, 124, 234101.	1.2	17
299	EXAFS Characterization of the Local Structure of Fe in FeZSM5 an Experimental and Theoretical Study. Physica Scripta, 2005, , 688.	1.2	2
300	Selective oxidation of methane over MoO/SiO: isolation of the kinetics of reactions occurring in the gas phase and on the surfaces of SiO and MoO. Journal of Catalysis, 2005, 231, 115-130.	3.1	39
301	Kinetic modeling of nitrous oxide decomposition on Fe-ZSM-5 based on parameters obtained from first-principles calculations. Journal of Catalysis, 2005, 233, 26-35.	3.1	68
302	The effects of zirconia morphology on methanol synthesis from CO and H <sub>2</sub> over Cu/ZrO <sub>2</sub> Cu/ZrO <sub>2</sub> catalystsPart I. Steady-state studies. Journal of Catalysis, 2005, 233, 198-209.	3.1	225
303	The effects of zirconia morphology on methanol synthesis from CO and H <sub>2</sub> over Cu/ZrO <sub>2</sub> catalystsPart II. Transient-response infrared studies. Journal of Catalysis, 2005, 233, 210-220.	3.1	103
304	A High-Yield, Liquid-Phase Approach for the Partial Oxidation of Methane to Methanol using SO <sub>3</sub> as the Oxidant. Advanced Synthesis and Catalysis, 2005, 347, 1203-1206.	2.1	19
305	Comprehensive DFT Study of Nitrous Oxide Decomposition over Fe-ZSM-5.. ChemInform, 2005, 36, no.	0.1	0
306	Quantitative analysis of hydrogen peroxide by <sup>1</sup> H NMR spectroscopy. Analytical and Bioanalytical Chemistry, 2005, 381, 1289-1293.	1.9	63

#	ARTICLE	IF	CITATIONS
307	Efficient methods for finding transition states in chemical reactions: Comparison of improved dimer method and partitioned rational function optimization method. <i>Journal of Chemical Physics</i> , 2005, 123, 224101.	1.2	662
308	Oxidative Dehydrogenation of Propane over V <sub>2</sub> O <sub>5</sub> /MoO <sub>3</sub> /Al <sub>2</sub> O <sub>3</sub> and V <sub>2</sub> O <sub>5</sub> /Cr <sub>2</sub> O <sub>3</sub> /Al <sub>2</sub> O <sub>3</sub> : A Structural Characterization and Catalytic Function. <i>Journal of Physical Chemistry B</i> , 2005, 109, 8987-9000.	1.2	94
309	Platinum-Based Catalysts for the Hydroamination of Olefins with Sulfonamides and Weakly Basic Anilines. <i>Journal of the American Chemical Society</i> , 2005, 127, 12640-12646.	6.6	161
310	A Study of the Redox Properties of MoO <sub>x</sub> /SiO <sub>2</sub> . <i>Journal of Physical Chemistry B</i> , 2005, 109, 23419-23429.	1.2	41
311	In situ UV-Visible Spectroscopic Measurements of Kinetic Parameters and Active Sites for Catalytic Oxidation of Alkanes on Vanadium Oxides. <i>Journal of Physical Chemistry B</i> , 2005, 109, 2414-2420.	1.2	42
312	Comprehensive DFT Study of Nitrous Oxide Decomposition over Fe-ZSM-5. <i>Journal of Physical Chemistry B</i> , 2005, 109, 1857-1873.	1.2	176
313	A Study of the Mechanism and Kinetics of Cyclooctene Epoxidation Catalyzed by Iron(III) Tetrakis(pentafluorophenyl) Porphyrin. <i>Journal of the American Chemical Society</i> , 2005, 127, 8635-8643.	6.6	93
314	A Density Functional Theory Study of the Mechanism of Free Radical Generation in the System Vanadate/PCA/H <sub>2</sub> O <sub>2</sub> . <i>Journal of Physical Chemistry B</i> , 2005, 109, 17984-17992.	1.2	85
315	Liquid-phase oxidation of alkylaromatics by a H-atom transfer mechanism with a new heterogeneous CoSBA-15 catalyst. <i>Chemical Communications</i> , 2005, , 3736.	2.2	80
316	An in situ cell for characterization of solids by soft x-ray absorption. <i>Review of Scientific Instruments</i> , 2004, 75, 3242-3247.	0.6	54
317	Rate constants from the reaction path Hamiltonian. II. Nonseparable semiclassical transition state theory. <i>Journal of Chemical Physics</i> , 2004, 121, 4461-4466.	1.2	17
318	Effects of additives on the activity and selectivity of supported vanadia catalysts for the oxidative dehydrogenation of propane. <i>Studies in Surface Science and Catalysis</i> , 2004, 147, 679-684.	1.5	1
319	Effects of molybdena on the catalytic properties of vanadia domains supported on alumina for oxidative dehydrogenation of propane. <i>Journal of Catalysis</i> , 2004, 221, 491-499.	3.1	131
320	Application of In Situ Surface-Enhanced Raman Spectroscopy (SERS) to the Study of Citrate Oxidation on Silica-Supported Silver Nanoparticles. <i>Catalysis Letters</i> , 2004, 92, 93-99.	1.4	23
321	A growing string method for determining transition states: Comparison to the nudged elastic band and string methods. <i>Journal of Chemical Physics</i> , 2004, 120, 7877-7886.	1.2	293
322	Direct Sulfonation of Methane to Methanesulfonic Acid by Sulfur Trioxide Catalyzed by Cerium(IV) Sulfate in the Presence of Molecular Oxygen. <i>Advanced Synthesis and Catalysis</i> , 2004, 346, 913-916.	2.1	23
323	Pt-Ag Catalyst System for Hydroarylations with Unactivated Arenes and Olefins. <i>ChemInform</i> , 2004, 35, no.	0.1	0
324	Catalyzed sulfonation of methane to methanesulfonic acid. <i>Journal of Molecular Catalysis A</i> , 2004, 211, 59-65.	4.8	21

#	ARTICLE	IF	CITATIONS
325	Nitrous oxide decomposition and surface oxygen formation on Fe-ZSM-5. <i>Journal of Catalysis</i> , 2004, 224, 148-155.	3.1	106
326	Methanol formation on Fe/Al-MFI via the oxidation of methane by nitrous oxide. <i>Journal of Catalysis</i> , 2004, 225, 300-306.	3.1	137
327	Direct oxidation of methane to acetic acid catalyzed by Pd <sup>2+</sup> and Cu <sup>2+</sup> in the presence of molecular oxygen. <i>Chemical Communications</i> , 2004, , 1948.	2.2	51
328	Rate constants from the reaction path Hamiltonian. I. Reactive flux simulations for dynamically correct rates. <i>Journal of Chemical Physics</i> , 2004, 121, 4453-4460.	1.2	24
329	Density Functional Theory Investigations of the Direct Oxidation of Methane on an Fe-Exchanged Zeolite. <i>Journal of Physical Chemistry B</i> , 2004, 108, 4362-4368.	1.2	45
330	Extent of Reduction of Vanadium Oxides during Catalytic Oxidation of Alkanes Measured by in-Situ UV-Visible Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2004, 108, 2345-2353.	1.2	84
331	Effects of Precursor Composition on the Local Structure of Cu Dispersed on Mesoporous Silica: A Detailed X-ray Absorption Spectroscopy Study. <i>Journal of Physical Chemistry B</i> , 2004, 108, 18421-18434.	1.2	36
332	Atomic Level Control over Surface Species via a Molecular Precursor Approach: Isolated Cu(I) Sites and Cu Nanoparticles Supported on Mesoporous Silica. <i>Journal of the American Chemical Society</i> , 2004, 126, 10864-10866.	6.6	58
333	Challenges for the application of quantum chemical calculations to problems in catalysis. <i>Molecular Physics</i> , 2004, 102, 319-329.	0.8	13
334	X-ray Absorption Fine Structure Analysis of the Local Environment of Fe in Fe/Al-MFI. <i>Journal of Physical Chemistry B</i> , 2004, 108, 8970-8975.	1.2	39
335	Methanol formation on Fe/Al-MFI via the oxidation of methane by nitrous oxide. <i>Journal of Catalysis</i> , 2004, 225, 300-300.	3.1	4
336	Pt-Ag Catalyst System for Hydroarylations with Unactivated Arenes and Olefins. <i>Organometallics</i> , 2004, 23, 4169-4171.	1.1	101
337	Synthesis of Trifluoromethanesulfonic Acid from CHF <sub>3</sub> . <i>Organic Process Research and Development</i> , 2004, 8, 660-662.	1.3	14
338	Synthesis of methanesulfonic acid and acetic acid by the direct sulfonation or carboxylation of methane. <i>Studies in Surface Science and Catalysis</i> , 2004, , 523-528.	1.5	1
339	Fast methods for resumming matrix polynomials and Chebyshev matrix polynomials. <i>Journal of Computational Physics</i> , 2004, 194, 575-587.	1.9	16
340	The Impact of Nanoscience on Heterogeneous Catalysis. <i>Science</i> , 2003, 299, 1688-1691.	6.0	2,263
341	Title is missing!. <i>Angewandte Chemie</i> , 2003, 115, 3098-3101.	1.6	9
342	Title is missing!. <i>Angewandte Chemie</i> , 2003, 115, 1049-1051.	1.6	14

#	ARTICLE	IF	CITATIONS
343	Title is missing!. <i>Angewandte Chemie</i> , 2003, 115, 3036-3036.	1.6	0
344	A High-Yield Approach to the Sulfonation of Methane to Methanesulfonic Acid Initiated by H <sub>2</sub> O <sub>2</sub> and a Metal Chloride. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 2990-2993.	7.2	45
345	Direct Liquid-Phase Sulfonation of Methane to Methanesulfonic Acid by SO <sub>3</sub> in the Presence of a Metal Peroxide. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 1019-1021.	7.2	40
346	Direct Liquid-Phase Sulfonation of Methane to Methanesulfonic Acid by SO <sub>3</sub> in the Presence of a Metal Peroxide. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 2930-2930.	7.2	0
347	Direct Sulfonation of Methane at Low Pressure to Methanesulfonic Acid in the Presence of Potassium Peroxydiphosphate as the Initiator. <i>Organic Process Research and Development</i> , 2003, 7, 161-163.	1.3	15
348	Effects of O <sub>2</sub> Concentration on the Rate and Selectivity in Oxidative Dehydrogenation of Ethane Catalyzed by Vanadium Oxide: Implications for O <sub>2</sub> Staging and Membrane Reactors. <i>Industrial &amp; Engineering Chemistry Research</i> , 2003, 42, 5462-5466.	1.8	16
349	Direct Sulfonation of Methane to Methanesulfonic Acid with SO <sub>2</sub> Using Ca Salts as Promoters. <i>Journal of the American Chemical Society</i> , 2003, 125, 4406-4407.	6.6	38
350	Synthesis of Mixed Acid Anhydrides from Methane and Carbon Dioxide in Acid Solvents. <i>Organic Letters</i> , 2003, 5, 3193-3196.	2.4	45
351	Synthesis and Study of Heterobimetallic Complexes Supported by a Ferrocene-Based Bisphosphine-Diamine Ligand. <i>Organometallics</i> , 2003, 22, 2855-2861.	1.1	16
352	X-ray Absorption Fine Structure Characterization of the Local Structure of Fe in Fe-ZSM-5. <i>Journal of Physical Chemistry B</i> , 2003, 107, 11843-11851.	1.2	87
353	A Novel Method for the Direct Sulfonation of CH <sub>4</sub> with SO <sub>3</sub> in the Presence of KO <sub>2</sub> and a Promoter. <i>Organic Process Research and Development</i> , 2003, 7, 754-757.	1.3	8
354	In situ UV-visible assessment of extent of reduction during oxidation reactions on oxide catalysts. <i>Chemical Communications</i> , 2003, , 2082.	2.2	20
355	Direct catalytic sulfonation of methane with SO <sub>2</sub> to methanesulfonic acid (MSA) in the presence of molecular O <sub>2</sub> . <i>Chemical Communications</i> , 2003, , 1590.	2.2	20
356	Biasing a transition state search to locate multiple reaction pathways. <i>Journal of Chemical Physics</i> , 2003, 118, 9533-9541.	1.2	28
357	Improved Fermi operator expansion methods for fast electronic structure calculations. <i>Journal of Chemical Physics</i> , 2003, 119, 4117-4125.	1.2	85
358	Density Functional Theory Study of Nitrous Oxide Decomposition over Fe- and Co-ZSM-5. <i>Journal of Physical Chemistry B</i> , 2002, 106, 7059-7064.	1.2	100
359	Effects of Solvent Acidity on the Free-Radical-Initiated Synthesis of Methanesulfonic Acid from CH <sub>4</sub> and SO <sub>3</sub> . <i>Industrial &amp; Engineering Chemistry Research</i> , 2002, 41, 5901-5905.	1.8	18
360	A Density Functional Theory Study of the Oxidation of Methanol to Formaldehyde over Vanadia Supported on Silica, Titania, and Zirconia. <i>Journal of Physical Chemistry B</i> , 2002, 106, 7832-7838.	1.2	98

#	ARTICLE	IF	CITATIONS
361	Synthesis, Characterization, and Catalytic Performance of Single-Site Iron(III) Centers on the Surface of SBA-15 Silica. <i>Journal of the American Chemical Society</i> , 2002, 124, 13194-13203.	6.6	207
362	Ethane Oxidative Dehydrogenation Pathways on Vanadium Oxide Catalysts. <i>Journal of Physical Chemistry B</i> , 2002, 106, 5421-5427.	1.2	114
363	Fast evaluation of a linear number of local exchange matrices. <i>Chemical Physics Letters</i> , 2002, 358, 43-50.	1.2	19
364	Oxidative Dehydrogenation of Propane over Vanadia-Magnesia Catalysts Prepared by Thermolysis of $\text{OV}(\text{OtBu})_3$ in the Presence of Nanocrystalline $\text{MgO}$ . <i>Journal of Catalysis</i> , 2002, 206, 49-59.	3.1	108
365	Effect of Catalyst Structure on Oxidative Dehydrogenation of Ethane and Propane on Alumina-Supported Vanadia. <i>Journal of Catalysis</i> , 2002, 208, 139-149.	3.1	298
366	Studies of $\text{N}_2\text{O}$ Adsorption and Decomposition on $\text{Fe-ZSM-5}$ . <i>Journal of Catalysis</i> , 2002, 209, 151-158.	3.1	92
367	The Relationship between the Electronic and Redox Properties of Dispersed Metal Oxides and Their Turnover Rates in Oxidative Dehydrogenation Reactions. <i>Journal of Catalysis</i> , 2002, 209, 35-42.	3.1	255
368	Effects of Zirconia Phase on the Synthesis of Methanol over Zirconia-Supported Copper. <i>Catalysis Letters</i> , 2002, 80, 63-68.	1.4	152
369	Cadmium Solid State NMR Studies of Cadmium-Exchanged Zeolites. <i>Catalysis Letters</i> , 2002, 80, 19-24.	1.4	4
370	Title is missing!. <i>Topics in Catalysis</i> , 2002, 20, 97-105.	1.3	82
371	Investigation of $\text{CO}$ and $\text{CO}_2$ Adsorption on Tetragonal and Monoclinic Zirconia. <i>Langmuir</i> , 2001, 17, 4297-4303.	1.6	415
372	Isotopic Tracer Studies of Reaction Pathways for Propane Oxidative Dehydrogenation on Molybdenum Oxide Catalysts. <i>Journal of Physical Chemistry B</i> , 2001, 105, 646-653.	1.2	79
373	Catalysis Research of Relevance to Carbon Management: Progress, Challenges, and Opportunities. <i>Chemical Reviews</i> , 2001, 101, 953-996.	23.0	1,311
374	An Experimental and Density Functional Theory Study of the Interactions of $\text{CH}_4$ with $\text{H-ZSM-5}$ . <i>Journal of Physical Chemistry A</i> , 2001, 105, 10454-10461.	1.1	42
375	Effects of Temperature on the Raman Spectra and Dispersed Oxides. <i>Journal of Physical Chemistry B</i> , 2001, 105, 5144-5152.	1.2	115
376	$\text{K}_2\text{S}_2\text{O}_8$ -Initiated Sulfonation of Methane to Methanesulfonic Acid. <i>Industrial &amp; Engineering Chemistry Research</i> , 2001, 40, 736-742.	1.8	28
377	Structure and Properties of Oxidative Dehydrogenation Catalysts Based on $\text{MoO}_3/\text{Al}_2\text{O}_3$ . <i>Journal of Catalysis</i> , 2001, 198, 232-242.	3.1	265
378	An in Situ Infrared Study of Dimethyl Carbonate Synthesis from Carbon Dioxide and Methanol over Zirconia. <i>Journal of Catalysis</i> , 2001, 204, 339-347.	3.1	188

#	ARTICLE	IF	CITATIONS
379	Catalytic Properties of Supported MoO <sub>3</sub> Catalysts for Oxidative Dehydrogenation of Propane. <i>Studies in Surface Science and Catalysis</i> , 2001, 136, 507-512.	1.5	8
380	Molecular Design of Highly Active Methanol Synthesis Catalysts. <i>Studies in Surface Science and Catalysis</i> , 2001, 136, 13-19.	1.5	13
381	The effects of synthesis and pretreatment conditions on the bulk structure and surface properties of zirconia. <i>Journal of Molecular Catalysis A</i> , 2000, 163, 27-42.	4.8	180
382	Title is missing!. <i>Catalysis Letters</i> , 2000, 70, 137-143.	1.4	42
383	Structure and Properties of Zirconia-Supported Molybdenum Oxide Catalysts for Oxidative Dehydrogenation of Propane. <i>Journal of Catalysis</i> , 2000, 189, 421-430.	3.1	163
384	Kinetic Isotopic Effects in Oxidative Dehydrogenation of Propane on Vanadium Oxide Catalysts. <i>Journal of Catalysis</i> , 2000, 192, 197-203.	3.1	152
385	Role of Hydrogen Spillover in Methanol Synthesis over Cu/ZrO <sub>2</sub> . <i>Journal of Catalysis</i> , 2000, 193, 207-223.	3.1	207
386	Thermolytic Molecular Precursor Route to Active and Selective Vanadia-Zirconia Catalysts for the Oxidative Dehydrogenation of Propane. <i>Journal of Catalysis</i> , 2000, 194, 431-444.	3.1	54
387	Site Availability and Competitive Siting of Divalent Metal Cations in ZSM-5. <i>Journal of Catalysis</i> , 2000, 194, 278-285.	3.1	62
388	Alkali Effects on Molybdenum Oxide Catalysts for the Oxidative Dehydrogenation of Propane. <i>Journal of Catalysis</i> , 2000, 195, 244-252.	3.1	98
389	Theoretical Studies of the Coordination and Stability of Divalent Cations in ZSM-5. <i>Journal of Physical Chemistry B</i> , 2000, 104, 9987-9992.	1.2	81
390	Structural Characterization of Molybdenum Oxide Supported on Zirconia. <i>Journal of Physical Chemistry B</i> , 2000, 104, 10059-10068.	1.2	116
391	Surface mobility and slip of polybutadiene melts in shear flow. <i>Journal of Rheology</i> , 2000, 44, 549-567.	1.3	39
392	Density Functional Theory Calculations of the Oxidative Dehydrogenation of Propane on the (010) Surface of V <sub>2</sub> O <sub>5</sub> . <i>Journal of Physical Chemistry B</i> , 2000, 104, 12250-12255.	1.2	74
393	Effects of Support Composition and Pretreatment Conditions on the Structure of Vanadia Dispersed on SiO <sub>2</sub> , Al <sub>2</sub> O <sub>3</sub> , TiO <sub>2</sub> , ZrO <sub>2</sub> , and HfO <sub>2</sub> . <i>Journal of Physical Chemistry B</i> , 2000, 104, 1516-1528.	1.2	180
394	Density Functional Theory Study of Proton Mobility in Zeolites: Proton Migration and Hydrogen Exchange in ZSM-5. <i>Journal of Physical Chemistry B</i> , 2000, 104, 6998-7011.	1.2	130
395	Effects of Hydration and Dehydration on the Structure of Silica-Supported Vanadia Species. <i>Langmuir</i> , 2000, 16, 7162-7167.	1.6	101
396	Water-Assisted Tetragonal-to-Monoclinic Phase Transformation of ZrO <sub>2</sub> at Low Temperatures. <i>Chemistry of Materials</i> , 2000, 12, 2442-2447.	3.2	112

#	ARTICLE	IF	CITATIONS
397	Kinetics and Mechanism of Oxidative Dehydrogenation of Propane on Vanadium, Molybdenum, and Tungsten Oxides. <i>Journal of Physical Chemistry B</i> , 2000, 104, 1292-1299.	1.2	276
398	NMR applied to zeolite synthesis. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 1999, 158, 221-234.	2.3	27
399	Dynamic Monte-Carlo and mean-field study of the effect of strong adsorption sites on self-diffusion in zeolites. <i>Chemical Engineering Science</i> , 1999, 54, 3455-3463.	1.9	67
400	Structure and Catalytic Properties of Supported Vanadium Oxides: Support Effects on Oxidative Dehydrogenation Reactions. <i>Journal of Catalysis</i> , 1999, 181, 205-216.	3.1	573
401	NO Reduction by CH <sub>4</sub> in the Presence of O <sub>2</sub> over Pd-H-ZSM-5. <i>Journal of Catalysis</i> , 1999, 181, 189-204.	3.1	100
402	A Mechanistic Study of Methanol Decomposition over Cu/SiO <sub>2</sub> , ZrO <sub>2</sub> /SiO <sub>2</sub> , and Cu/ZrO <sub>2</sub> /SiO <sub>2</sub> . <i>Journal of Catalysis</i> , 1999, 184, 357-376.	3.1	189
403	Isotopic Tracer and Kinetic Studies of Oxidative Dehydrogenation Pathways on Vanadium Oxide Catalysts. <i>Journal of Catalysis</i> , 1999, 186, 325-333.	3.1	295
404	The Dynamics of Oxygen Exchange with Zirconia-Supported PdO. <i>Journal of Catalysis</i> , 1999, 185, 213-218.	3.1	27
405	Al Next Nearest Neighbor, Ring Occupation, and Proximity Statistics in ZSM-5. <i>Journal of Catalysis</i> , 1999, 186, 222-227.	3.1	97
406	Investigations of the State of Fe in H <sub>2</sub> ZSM-5. <i>Journal of Catalysis</i> , 1999, 186, 242-253.	3.1	388
407	Isotopic Studies of Methane Oxidation Pathways on PdO Catalysts. <i>Journal of Catalysis</i> , 1999, 188, 132-139.	3.1	92
408	An in situ infrared study of NO reduction by C <sub>3</sub> H <sub>8</sub> over Fe-ZSM-5. <i>Catalysis Letters</i> , 1999, 63, 233-240.	1.4	115
409	Title is missing!. <i>Topics in Catalysis</i> , 1999, 9, 207-213.	1.3	47
410	Vanadyl-tert-Butoxy Orthosilicate, OV[OSi(OtBu) <sub>3</sub> ] <sub>3</sub> : A Model for Isolated Vanadyl Sites on Silica and a Precursor to Vanadia-Silica Xerogels. <i>Chemistry of Materials</i> , 1999, 11, 2966-2973.	3.2	79
411	Influence of Occupancy and Pore Network Topology on Tracer and Transport Diffusion in Zeolites. , 1999, , 200-207.		1
412	Effect of topology and molecular occupancy on self-diffusion in lattice models of zeolites—Monte-Carlo simulations. <i>Chemical Engineering Science</i> , 1998, 53, 2053-2061.	1.9	71
413	Title is missing!. <i>Catalysis Letters</i> , 1998, 54, 105-111.	1.4	18
414	Title is missing!. <i>Catalysis Letters</i> , 1998, 50, 135-139.	1.4	53



#	ARTICLE	IF	CITATIONS
415	A Study of the Dynamics of Pd Oxidation and PdO Reduction by H <sub>2</sub> and CH <sub>4</sub> . Journal of Catalysis, 1998, 176, 125-135.	3.1	223
416	In Situ Infrared Study of Methanol Synthesis from H <sub>2</sub> /CO over Cu/SiO <sub>2</sub> and Cu/ZrO <sub>2</sub> /SiO <sub>2</sub> . Journal of Catalysis, 1998, 178, 153-173.	3.1	203
417	Structure and properties of vanadium oxide-zirconia catalysts for propane oxidative dehydrogenation. Journal of Catalysis, 1998, 177, 343-351.	3.1	267
418	Near-surface dynamics of sheared polymer melts using ATR/FTIR. AIChE Journal, 1998, 44, 701-710.	1.8	12
419	A Study of the Structure of Vanadium Oxide Dispersed on Zirconia. Journal of Physical Chemistry B, 1998, 102, 7000-7007.	1.2	66
420	A Density Functional Theory Study of the Interactions of H <sub>2</sub> O with H <sup>+</sup> -ZSM-5, Cu <sup>+</sup> -ZSM-5, and Co <sup>+</sup> -ZSM-5. Journal of Physical Chemistry A, 1998, 102, 7498-7504.	1.1	56
421	Single-input double-tuned circuit for double resonance nuclear magnetic resonance experiments. Review of Scientific Instruments, 1998, 69, 477-478.	0.6	15
422	Density Functional Theory Calculations of the Effects of Local Composition and Defect Structure on the Proton Affinity of H <sup>+</sup> -ZSM-5. Journal of Physical Chemistry B, 1997, 101, 10058-10064.	1.2	55
423	<sup>65</sup> Cu NMR Spectroscopy of Cu-Exchanged ZSM-5 Catalysts. Journal of Physical Chemistry B, 1997, 101, 1869-1871.	1.2	28
424	In-Situ Infrared Study of Methanol Synthesis from H <sub>2</sub> /CO <sub>2</sub> over Cu/SiO <sub>2</sub> and Cu/ZrO <sub>2</sub> /SiO <sub>2</sub> . Journal of Catalysis, 1997, 172, 222-237.	3.1	311
425	Investigations of the Dispersion of Pd in H-ZSM-5. Journal of Catalysis, 1997, 172, 453-462.	3.1	126
426	NO Adsorption, Desorption, and Reduction by CH <sub>4</sub> over Mn-ZSM-5. Journal of Catalysis, 1997, 170, 390-401.	3.1	82
427	Diffusion and reaction in ZSM-5 studied by dynamic Monte Carlo. Chemical Engineering Science, 1997, 52, 2265-2276.	1.9	44
428	Raman studies of peroxide formation, decomposition, and reduction on Ba/MgO. Catalysis Letters, 1996, 36, 15-19.	1.4	15
429	Computer simulation of the interactions of tetraalkylammonium cations with ZSM-5 and ZSM-11. Microporous Materials, 1996, 7, 187-199.	1.6	18
430	Local Spin Density Functional Theory Study of Copper Ion-Exchanged ZSM-5. The Journal of Physical Chemistry, 1996, 100, 4173-4179.	2.9	103
431	Investigation of the dynamics of benzene in silicalite using transition-state theory. Studies in Surface Science and Catalysis, 1995, 98, 240-241.	1.5	5
432	Surface interactions in a shear field. AIChE Journal, 1995, 41, 1266-1272.	1.8	10

#	ARTICLE	IF	CITATIONS
433	The influence of metal oxides on the activity and selectivity of transition metal catalysts. <i>Journal of Molecular Catalysis A</i> , 1995, 100, 1-11.	4.8	32
434	Dynamics of flow-induced surface exchange. <i>Industrial &amp; Engineering Chemistry Research</i> , 1995, 34, 3336-3341.	1.8	8
435	Electronic Structure Calculations of Ammonia Adsorption in H-ZSM-5 Zeolites. <i>The Journal of Physical Chemistry</i> , 1995, 99, 1505-1515.	2.9	63
436	Investigation of the dynamics of benzene in silicalite using Transition-State Theory. <i>The Journal of Physical Chemistry</i> , 1994, 98, 11948-11961.	2.9	93
437	Electron Paramagnetic Resonance Studies of Copper Ion-Exchanged ZSM-5. <i>The Journal of Physical Chemistry</i> , 1994, 98, 11533-11540.	2.9	302
438	Raman investigations of NH <sub>3</sub> adsorption on TiO <sub>2</sub> , Nb <sub>2</sub> O <sub>5</sub> , and Nb <sub>2</sub> O <sub>5</sub> /TiO <sub>2</sub> . <i>Catalysis Letters</i> , 1994, 24, 1-13.	1.4	39
439	Estimates of rate coefficients for elementary processes occurring during Fischer-Tropsch synthesis over Ru/TiO <sub>2</sub> . <i>Journal of Catalysis</i> , 1994, 146, 237-248.	3.1	83
440	Adsorption and decomposition of CH <sub>3</sub> NH <sub>2</sub> on Mo(100)-c(2 × 2)N. <i>Surface Science</i> , 1994, 316, 267-276.	0.8	22
441	The effect of electric field gradient asymmetry on motionally averaged spin-1 powder patterns. <i>Solid State Nuclear Magnetic Resonance</i> , 1993, 2, 1-10.	1.5	3
442	The activity of transition metal nitrides for hydrotreating quinoline and thiophene. <i>Catalysis Letters</i> , 1993, 21, 11-18.	1.4	45
443	Catalytic hydrotreating of indole, benzothiophene, and benzofuran over Mo <sub>2</sub> N. <i>Catalysis Letters</i> , 1993, 18, 1-8.	1.4	91
444	Decomposition and reduction of NO on transition metal surfaces: bond order conservation Morse potential analysis. <i>Surface Science</i> , 1993, 289, 127-138.	0.8	92
445	Raman studies of the structure of niobium oxide/titanium oxide (Nb <sub>2</sub> O <sub>5</sub> .TiO <sub>2</sub> ). <i>The Journal of Physical Chemistry</i> , 1993, 97, 12178-12185.	2.9	123
446	Prediction of adsorption of aromatic hydrocarbons in silicalite from grand canonical Monte Carlo simulations with biased insertions. <i>The Journal of Physical Chemistry</i> , 1993, 97, 13742-13752.	2.9	366
447	A Tribute to Heinz Heinemann. <i>Catalysis Reviews - Science and Engineering</i> , 1993, 35, v-vi.	5.7	0
448	Interactions of H <sub>2</sub> and NH <sub>3</sub> with Mo(100) and Mo(100)-c(2 × 2) N surfaces. <i>Surface Science</i> , 1992, 278, 353-363.	0.8	27
449	Oxygen-assisted cleavage of O-H, Ni-H, and C-H bonds on transition metal surfaces: bond-order-conservation-Morse-potential analysis. <i>Surface Science</i> , 1992, 268, 397-405.	0.8	60
450	Molecular dynamics studies of butane and hexane in silicalite. <i>The Journal of Physical Chemistry</i> , 1992, 96, 1051-1060.	2.9	244

#	ARTICLE	IF	CITATIONS
451	The role of C2 intermediates in Fischer-Tropsch synthesis over ruthenium. <i>Catalysis Letters</i> , 1992, 14, 305-313.	1.4	32
452	Quantitative structural analysis of dispersed vanadia species in TiO <sub>2</sub> (anatase)-supported V <sub>2</sub> O <sub>5</sub> . <i>Journal of Catalysis</i> , 1992, 134, 479-491.	3.1	259
453	The effects of structure on the catalytic activity and selectivity of V <sub>2</sub> O <sub>5</sub> /TiO <sub>2</sub> for the reduction of NO by NH <sub>3</sub> . <i>Journal of Catalysis</i> , 1992, 134, 492-505.	3.1	241
454	Molecular Simulations of Methane Adsorption in Silicalite. <i>Molecular Simulation</i> , 1991, 8, 73-92.	0.9	61
455	Monte Carlo simulations of the effect of pressure on isothermal and temperature-programmed desorption kinetics. <i>Surface Science</i> , 1991, 245, 213-224.	0.8	36
456	Synthesis and decomposition of ammonia on transition metal surfaces: bond-order-conservation-Morse-potential analysis. <i>Surface Science</i> , 1991, 259, L791-L796.	0.8	45
457	An analysis of methanol synthesis from CO and CO <sub>2</sub> on Cu and Pd surfaces by the bond-order-conservation-Morse-potential approach. <i>Surface Science</i> , 1991, 253, 386-394.	0.8	71
458	An analysis of Fischer-Tropsch synthesis by the bond-order-conservation-Morse-potential approach. <i>Surface Science</i> , 1991, 248, 359-368.	0.8	76
459	10 Reflections on the Current Status and Future Directions of Chemical Reaction Engineering. <i>Advances in Chemical Engineering</i> , 1991, 16, 205-226.	0.5	0
460	Synthesis and decomposition of ammonia on transition metal surfaces: bond-order-conservation-Morse-potential analysis. <i>Surface Science Letters</i> , 1991, 259, L791-L796.	0.1	2
461	A review of theoretical models of adsorption, diffusion, desorption, and reaction of gases on metal surfaces. <i>Surface Science Reports</i> , 1991, 13, 3-72.	3.8	208
462	Transition-state studies of xenon and sulfur hexafluoride diffusion in silicalite. <i>The Journal of Physical Chemistry</i> , 1991, 95, 8866-8878.	2.9	180
463	The effects of local structural relaxation on aluminum siting within H-ZSM-5. <i>Catalysis Letters</i> , 1991, 11, 209-217.	1.4	103
464	Studies on the mechanism of ZSM-5 formation. <i>Catalysis Letters</i> , 1991, 8, 305-316.	1.4	127
465	Laser Raman spectroscopy of NH <sub>3</sub> and ND <sub>3</sub> adsorbed on TiO <sub>2</sub> (anatase). <i>Catalysis Letters</i> , 1991, 11, 111-117.	1.4	17
466	The impact of catalyst science on catalyst design and development. <i>Chemical Engineering Science</i> , 1990, 45, 2013-2026.	1.9	12
467	Prediction of low occupancy sorption of alkanes in silicalite. <i>The Journal of Physical Chemistry</i> , 1990, 94, 1508-1516.	2.9	210
468	Molecular dynamics study of methane and xenon in silicalite. <i>The Journal of Physical Chemistry</i> , 1990, 94, 8232-8240.	2.9	258

#	ARTICLE	IF	CITATIONS
469	Laser Raman spectroscopy of supported vanadium oxide catalysts. <i>The Journal of Physical Chemistry</i> , 1990, 94, 4240-4246.	2.9	416
470	Analysis of the thermochemistry of C2 hydrocarbons on transition metal surfaces using a refined BOC-MP approach. <i>Surface Science</i> , 1990, 235, 343-350.	0.8	20
471	Surface Chemistry of Carbonaceous Species. <i>Studies in Surface Science and Catalysis</i> , 1989, 48, 91-109.	1.5	8
472	Applications of NMR Spectroscopy to the Study of Zeolite Synthesis. <i>ACS Symposium Series</i> , 1989, , 66-82.	0.5	19
473	TPD and IR spectroscopic studies of CO, CO2 and H2 adsorption on LaCrO3. <i>Applied Surface Science</i> , 1989, 37, 353-366.	3.1	9
474	Magic-angle-spinning NMR spectroscopy of gels. <i>Journal of Magnetic Resonance</i> , 1989, 81, 217-219.	0.5	2
475	Surface reactivity of reduced LaFeO3 as studied by TPD and IR spectroscopies of CO, CO2 and H2. <i>Journal of Materials Science</i> , 1989, 24, 4437-4442.	1.7	29
476	An analysis of formic acid decomposition on metal surfaces by the bond-order-conservation-Morse-potential approach. <i>Surface Science</i> , 1989, 222, 371-382.	0.8	28
477	Monte carlo simulation of temperature-programmed desorption of coadsorbed species. <i>Surface Science</i> , 1989, 224, 451-475.	0.8	22
478	NMR studies of model hydrodenitrogenation catalysis: acetonitrile hydrogenation on .gamma.-dimolybdenum mononitride. <i>The Journal of Physical Chemistry</i> , 1989, 93, 5859-5865.	2.9	20
479	Surface behaviour of reduced LaCoO3 as studied by TPD of CO, CO2 and H2 probes and by XPS. <i>Applied Surface Science</i> , 1988, 31, 301-316.	3.1	97
480	Characterization of CO adsorbed on ?-Mo2N by NMR spectroscopy. <i>Catalysis Letters</i> , 1988, 1, 207-212.	1.4	7
481	A monte carlo model for the simulation of temperature-programmed desorption spectra. <i>Surface Science</i> , 1988, 206, 101-123.	0.8	43
482	The thermochemistry of C2 hydrocarbons on transition metal surfaces: The bond-order-conservation approach. <i>Surface Science</i> , 1988, 205, 492-512.	0.8	44
483	The influence of preparation chemistry on the phase distribution of silica-supported titania. <i>Applied Catalysis</i> , 1987, 32, 315-326.	1.1	48
484	Influence of particle size on carbon monoxide hydrogenation over silica- and lanthana-supported rhodium. <i>Applied Catalysis</i> , 1987, 34, 289-310.	1.1	48
485	The effects of titania and alumina overlayers on the hydrogenation of CO over rhodium. <i>Journal of the Chemical Society Faraday Transactions I</i> , 1987, 83, 2061.	1.0	47
486	Temperature-programmed desorption study of the interactions of H2, CO and CO2 with LaMnO3. <i>Journal of the Chemical Society Faraday Transactions I</i> , 1987, 83, 3149.	1.0	21

#	ARTICLE	IF	CITATIONS
487	Raman study of the preparation of silica-supported titania from titanium tetrachloride and hydrogen chloride. <i>Langmuir</i> , 1987, 3, 111-116.	1.6	44
488	Effect of promoting Rh/SiO <sub>2</sub> with TiO <sub>2</sub> on the reduction of nitric oxide. <i>Applied Catalysis</i> , 1986, 20, 109-122.	1.1	13
489	Studies of fischer-Tropsch synthesis over a fused iron catalyst. <i>Applied Catalysis</i> , 1986, 20, 145-162.	1.1	18
490	Influence of ethylene on the hydrogenation of carbon monoxide over ruthenium. <i>The Journal of Physical Chemistry</i> , 1986, 90, 4797-4805.	2.9	100
491	CO hydrogenation over rhodium supported on SiO <sub>2</sub> , La <sub>2</sub> O <sub>3</sub> , Nd <sub>2</sub> O <sub>3</sub> and Sm <sub>2</sub> O <sub>3</sub> . <i>Applied Catalysis</i> , 1986, 21, 157-168.	1.1	73
492	A theoretical model for the performance of bubble-column reactors used for Fischer-Tropsch synthesis. <i>Chemical Engineering Science</i> , 1985, 40, 1665-1677.	1.9	33
493	Experimental and theoretical studies of Fischer-Tropsch synthesis over ruthenium in a bubble-column reactor. <i>Chemical Engineering Science</i> , 1985, 40, 1917-1924.	1.9	12
494	On-line analysis of Fischer-Tropsch synthesis products. <i>Industrial &amp; Engineering Chemistry Fundamentals</i> , 1984, 23, 252-256.	0.7	17
495	In Situ Measurement of Resist Dissolution with a Psi-Meter. <i>Journal of the Electrochemical Society</i> , 1984, 131, 2200-2201.	1.3	4
496	The influence of metal-support interactions on the catalytic properties of Pd/La <sub>2</sub> O <sub>3</sub> . <i>Applications of Surface Science</i> , 1984, 19, 315-329.	1.0	28
497	Effects of Lewis acid catalysts on the hydrogenation and cracking of three-ring aromatic and hydroaromatic structures related to coal. <i>Fuel</i> , 1984, 63, 469-476.	3.4	44
498	A mathematical model for spin coating of polymer resists. <i>Journal of Applied Physics</i> , 1984, 56, 1199-1206.	1.1	225
499	Effects of mass transfer on the performance of slurry reactors used for fischer-tropsch synthesis. <i>Chemical Engineering Science</i> , 1983, 38, 597-605.	1.9	49
500	An explanation for deviations of Fischer-Tropsch products from a Schulz-Flory distribution. <i>Industrial &amp; Engineering Chemistry Process Design and Development</i> , 1983, 22, 678-681.	0.6	37
501	Effects of Lewis acid catalysts on the hydrogenation and cracking of two-ring aromatic and hydroaromatic structures related to coal. <i>Fuel</i> , 1982, 61, 745-754.	3.4	17
502	Plasma polymerization of tetrafluoroethylene in a field-free zone. <i>Journal of Applied Polymer Science</i> , 1982, 27, 3965-3985.	1.3	25
503	Catalytic Synthesis of Hydrocarbons over Group VIII Metals. A Discussion of the Reaction Mechanism. <i>Catalysis Reviews - Science and Engineering</i> , 1981, 23, 203-232.	5.7	364
504	Gas chromatographic determination of gases formed in catalytic reduction of nitric oxide. <i>Analytical Chemistry</i> , 1981, 53, 817-820.	3.2	18

#	ARTICLE	IF	CITATIONS
505	<title>Applications Of Fourier Transform Infrared Spectroscopy To The Study Of Catalytic Reactions</title>. , 1981, , .		0
506	Conversion of solvent-refined coal to liquid products in the presence of Lewis acids. Fuel, 1981, 60, 52-58.	3.4	8
507	Effects of Lewis acid catalysts on the cleavage of aliphatic and aryl-aryl linkages in coal-related structures. Fuel, 1980, 59, 499-506.	3.4	45
508	Effects of zinc chloride on sulphur removal from coal-related structures. Fuel, 1980, 59, 507-510.	3.4	22
509	Polymerization of phosphazene crystal by plasma-exposure. Nature, 1980, 286, 693-694.	13.7	32
510	A Review of Recent Advances in Plasma Polymerization. ACS Symposium Series, 1979, , 1-33.	0.5	30
511	Plasma-Initiated Polymerization and Copolymerization of Liquid Vinyl Monomers. ACS Symposium Series, 1979, , 253-261.	0.5	11
512	Effects of zinc chloride on the cleavage of ether structures present in coal. Fuel, 1979, 58, 661-666.	3.4	39
513	Studies of CO desorption and reaction with H <sub>2</sub> on alumina-supported Ru. Journal of Catalysis, 1979, 57, 397-405.	3.1	121
514	Theoretical estimations of $\hat{\Gamma}^{\text{H}}\hat{A}^{\text{f,T}}$ , $\hat{\Gamma}^{\text{S}}\hat{A}^{\text{f,T}}$ , and $\hat{\Gamma}^{\text{G}}\hat{A}^{\text{f,T}}$ for Ca(O <sub>2</sub> ) <sub>2</sub> . Journal of Solid State Chemistry, 1979, 29, 97-100.	1.4	4
515	Characterization of Crystalline Poly(trioxane) and Poly(tetraoxane) Obtained through Plasma-Initiated Polymerization. ACS Symposium Series, 1979, , 263-274.	0.5	4
516	Plasma-initiated polymerization of methyl methacrylate. Journal of Polymer Science, Polymer Letters Edition, 1978, 16, 309-311.	0.4	56
517	Plasma-initiated solid-state polymerization of trioxane and tetraoxane. Journal of Polymer Science, Polymer Letters Edition, 1978, 16, 669-675.	0.4	14
518	Effect of alkali metal catalysts on gasification of coal char. Fuel, 1978, 57, 194-200.	3.4	240
519	An infrared study of NO and CO adsorption on a silica-supported Ru catalyst. Journal of Catalysis, 1977, 49, 332-344.	3.1	100
520	Infrared study of the reactions between NO and CO and NO and H <sub>2</sub> on a silica-supported Ru catalyst. Journal of Catalysis, 1977, 49, 345-355.	3.1	39
521	Synthesis of higher oxides of potassium in an electric discharge sustained in oxygen. Journal of Inorganic and Nuclear Chemistry, 1976, 38, 1943-1948.	0.5	2
522	Synthesis of higher oxides of lithium and calcium in an electric discharge sustained in oxygen. Journal of Inorganic and Nuclear Chemistry, 1976, 38, 1570-1571.	0.5	1

#	ARTICLE	IF	CITATIONS
523	Fundamentals of Plasma Polymerization. Journal of Macromolecular Science Part A, Chemistry, 1976, 10, 369-381.	0.4	30
524	A study of the performance and chemical characteristics of composite reverse osmosis membranes prepared by plasma polymerization of allylamine. Journal of Applied Polymer Science, 1975, 19, 1911-1930.	1.3	63
525	Microwave decomposition of toxic vapor simulants. Environmental Science & Technology, 1975, 9, 254-258.	4.6	17
526	Mass spectrometric study of ionic species present during the oxidation of CO and the decomposition of CO <sub>2</sub> in a rf discharge. Journal of Chemical Physics, 1974, 61, 666-671.	1.2	9
527	Formation of an amorphous powder during the polymerization of ethylene in a radio-frequency discharge. Journal of Applied Polymer Science, 1973, 17, 885-892.	1.3	124
528	A Model for the Kinetics of Oxygen Dissociation in a Microwave Discharge. Industrial & Engineering Chemistry Fundamentals, 1973, 12, 90-94.	0.7	23
529	Dissociation of oxygen in a radiofrequency electrical discharge. AIChE Journal, 1972, 18, 990-998.	1.8	40
530	Dynamic Boundary Layer Simulation of Pulsed CO <sub>2</sub> Electrolysis on a Copper Catalyst. ACS Energy Letters, 0, , 1181-1188.	8.8	61
531	Prof. Daniel E. Resasco associate editor of catalysis reviews. Catalysis Reviews - Science and Engineering, 0, , 1-1.	5.7	0