Dionisios G Vlachos

List of Publications by Year
in descending order

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444 papers	26,300 citations	4388 86 h-index	11052 137 g-index
464 all docs	464 docs citations	464 times ranked	17573 citing authors

#	Article	IF	Citations
1	Merocyanine 540 as an optical probe of transmembrane electrical activity in the heart. Science, 2003, 191, 485-487.	12.6	987
2	Insights into the Interplay of Lewis and BrÃ¸nsted Acid Catalysts in Glucose and Fructose Conversion to 5-(Hydroxymethyl)furfural and Levulinic Acid in Aqueous Media. Journal of the American Chemical Society, 2013, 135, 3997-4006.	13.7	586
3	Mechanistic Insights into the Electrochemical Reduction of CO₂ to CO on Nanostructured Ag Surfaces. ACS Catalysis, 2015, 5, 4293-4299.	11.2	476
4	Top ten fundamental challenges of biomass pyrolysis for biofuels. Energy and Environmental Science, 2012, 5, 7797.	30.8	474
5	Cycloaddition of Biomass-Derived Furans for Catalytic Production of Renewable p-Xylene. ACS Catalysis, 2012, 2, 935-939.	11.2	400
6	Using first principles to predict bimetallic catalysts for the ammonia decomposition reaction. Nature Chemistry, 2010, 2, 484-489.	13.6	381
7	An overview of spatial microscopic and accelerated kinetic Monte Carlo methods. Journal of Computer-Aided Materials Design, 2007, 14, 253-308.	0.7	376
8	Nickel supported on nitrogen-doped carbon nanotubes as hydrogen oxidation reaction catalyst in alkaline electrolyte. Nature Communications, 2016, 7, 10141.	12.8	368
9	Conversion of Xylose to Furfural Using Lewis and BrÃ¸nsted Acid Catalysts in Aqueous Media. ACS Catalysis, 2012, 2, 2022-2028.	11.2	312
10	A review on microcombustion: Fundamentals, devices and applications. Progress in Energy and Combustion Science, 2012, 38, 321-359.	31.2	307
11	Xylose Isomerization to Xylulose and its Dehydration to Furfural in Aqueous Media. ACS Catalysis, 2011, 1, 1724-1728.	11.2	301
12	Correlating Particle Size and Shape of Supported Ru/Î³-Al₂O₃ Catalysts with NH₃ Decomposition Activity. Journal of the American Chemical Society, 2009, 131, 12230-12239.	13.7	279
13	Molecular structure, morphology and growth mechanisms and rates of 5-hydroxymethyl furfural (HMF) derived humins. Green Chemistry, 2016, 18, 1983-1993.	9.0	276
14	Revealing pyrolysis chemistry for biofuels production: Conversion of cellulose to furans and small oxygenates. Energy and Environmental Science, 2012, 5, 5414-5424.	30.8	267
15	Production of Dimethylfuran from Hydroxymethylfurfural through Catalytic Transfer Hydrogenation with Ruthenium Supported on Carbon. ChemSusChem, 2013, 6, 1158-1162.	6.8	247
16	Mechanistic Insights into Metal Lewis Acid-Mediated Catalytic Transfer Hydrogenation of Furfural to 2-Methylfuran. ACS Catalysis, 2015, 5, 3988-3994.	11.2	244
17	DFT Study of Furfural Conversion to Furan, Furfuryl Alcohol, and 2-Methylfuran on Pd(111). ACS Catalysis, 2012, 2, 2496-2504.	11.2	232
18	Steam and dry reforming of methane on Rh: Microkinetic analysis and hierarchy of kinetic models. Journal of Catalysis, 2008, 259, 211-222.	6.2	223

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19	Liquid phase catalytic transfer hydrogenation of furfural over a Ru/C catalyst. Applied Catalysis A: General, 2014, 480, 17-24.	4.3	216
20	Plastic waste to fuels by hydrocracking at mild conditions. Science Advances, 2021, 7, .	10.3	214
21	Mechanistic Study of Alcohol Dehydration on Î³-Al₂O₃. ACS Catalysis, 2012, 2, 1846-1853.	11.2	199
22	Unraveling the Complexity of Catalytic Reactions via Kinetic Monte Carlo Simulation: Current Status and Frontiers. ACS Catalysis, 2012, 2, 2648-2663.	11.2	195
23	Binomial distribution based Ï„-leap accelerated stochastic simulation. Journal of Chemical Physics, 2005, 122, 024112.	3.0	184
24	Zeolite Growth by Addition of Subcolloidal Particles:Â Modeling and Experimental Validation. Chemistry of Materials, 2000, 12, 845-853.	6.7	179
25	Effect of hydrogen donor on liquid phase catalytic transfer hydrogenation of furfural over a Ru/RuO2/C catalyst. Journal of Molecular Catalysis A, 2014, 392, 223-228.	4.8	178
26	Selective Hydrodeoxygenation of Biomassâ€Derived Oxygenates to Unsaturated Hydrocarbons using Molybdenum Carbide Catalysts. ChemSusChem, 2013, 6, 798-801.	6.8	173
27	Coverage-Induced Conformational Effects on Activity and Selectivity: Hydrogenation and Decarbonylation of Furfural on Pd(111). ACS Catalysis, 2015, 5, 104-112.	11.2	172
28	A graph-theoretical kinetic Monte Carlo framework for on-lattice chemical kinetics. Journal of Chemical Physics, 2011, 134, 214115.	3.0	171
29	Structure of the Silica Phase Extracted from Silica/(TPA)OH Solutions Containing Nanoparticles. Journal of Physical Chemistry B, 2003, 107, 10006-10016.	2.6	164
30	Zeolite (MFI) Crystal Morphology Control Using Organic Structure-Directing Agents. Chemistry of Materials, 2004, 16, 5697-5705.	6.7	164
31	Growth of a faujasite-type zeolite membrane and its application in the separation of saturated/unsaturated hydrocarbon mixtures. Journal of Membrane Science, 2001, 184, 209-219.	8.2	161
32	DFT Study of the Waterâ€“Gas Shift Reaction and Coke Formation on Ni(111) and Ni(211) Surfaces. Journal of Physical Chemistry C, 2012, 116, 20281-20291.	3.1	157
33	Understanding solvent effects in the selective conversion of fructose to 5-hydroxymethyl-furfural: a molecular dynamics investigation. Physical Chemistry Chemical Physics, 2012, 14, 2637.	2.8	146
34	Thermodynamic Consistency in Microkinetic Development of Surface Reaction Mechanisms. Journal of Physical Chemistry B, 2003, 107, 12721-12733.	2.6	145
35	Hydrogenation of Ethylene and Dehydrogenation and Hydrogenolysis of Ethane on Pt(111) and Pt(211): A Density Functional Theory Study. Journal of Physical Chemistry C, 2010, 114, 4973-4982.	3.1	142
36	A DFT study of the acid-catalyzed conversion of 2,5-dimethylfuran and ethylene to p-xylene. Journal of Catalysis, 2013, 297, 35-43.	6.2	139

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37	Stability and performance of catalytic microreactors: Simulations of propane catalytic combustion on Pt. Chemical Engineering Science, 2008, 63, 1098-1116.	3.8	137
38	Spontaneous Formation of Silica Nanoparticles in Basic Solutions of Small Tetraalkylammonium Cations. Journal of Physical Chemistry B, 2004, 108, 12271-12275.	2.6	136
39	The Role of Ru and RuO₂ in the Catalytic Transfer Hydrogenation of 5â€Hydroxymethylfurfural for the Production of 2,5â€Dimethylfuran. ChemCatChem, 2014, 6, 848-856.	3.7	136
40	Mechanism of BrÃ¸nsted Acidâ€Catalyzed Glucose Dehydration. ChemSusChem, 2015, 8, 1334-1341.	6.8	135
41	Microkinetic Modeling for Water-Promoted CO Oxidation, Waterâ^'Gas Shift, and Preferential Oxidation of CO on Pt. Journal of Physical Chemistry B, 2004, 108, 15246-15258.	2.6	134
42	Vapor phase hydrodeoxygenation of furfural to 2-methylfuran on molybdenum carbide catalysts. Catalysis Science and Technology, 2014, 4, 2340.	4.1	132
43	Tandem Lewis acid/BrÃ¸nsted acid-catalyzed conversion of carbohydrates to 5-hydroxymethylfurfural using zeolite beta. Journal of Catalysis, 2016, 333, 149-161.	6.2	132
44	Effects of correlated parameters and uncertainty in electronic-structure-based chemical kinetic modelling. Nature Chemistry, 2016, 8, 331-337.	13.6	131
45	Câ€“O bond activation using ultralow loading of noble metal catalysts on moderately reducible oxides. Nature Catalysis, 2020, 3, 446-453.	34.4	131
46	Density Functional Theory-Computed Mechanisms of Ethylene and Diethyl Ether Formation from Ethanol on Î³-Al₂O₃(100). ACS Catalysis, 2013, 3, 1965-1975.	11.2	130
47	Role of Silanol Group in Sn-Beta Zeolite for Glucose Isomerization and Epimerization Reactions. ACS Catalysis, 2013, 3, 2294-2298.	11.2	128
48	Comparison of Homogeneous and Heterogeneous Catalysts for Glucoseâ€toâ€Fructose Isomerization in Aqueous Media. ChemSusChem, 2013, 6, 2369-2376.	6.8	128
49	Mechanisms for High Selectivity in the Hydrodeoxygenation of 5-Hydroxymethylfurfural over PtCo Nanocrystals. ACS Catalysis, 2016, 6, 4095-4104.	11.2	124
50	Structural analysis of humins formed in the BrÃ¸nsted acid catalyzed dehydration of fructose. Green Chemistry, 2018, 20, 997-1006.	9.0	123
51	Kinetics of Homogeneous BrÃ¸nsted Acid Catalyzed Fructose Dehydration and 5-Hydroxymethyl Furfural Rehydration: A Combined Experimental and Computational Study. ACS Catalysis, 2014, 4, 259-267.	11.2	122
52	Physical Basis for the Formation and Stability of Silica Nanoparticles in Basic Solutions of Monovalent Cations. Langmuir, 2005, 21, 8960-8971.	3.5	120
53	Pyrolytic conversion of cellulose to fuels: levoglucosan deoxygenation via elimination and cyclization within molten biomass. Energy and Environmental Science, 2012, 5, 7864.	30.8	119
54	Hierarchical Multiscale Mechanism Development for Methane Partial Oxidation and Reforming and for Thermal Decomposition of Oxygenates on Rh. Journal of Physical Chemistry B, 2005, 109, 16819-16835.	2.6	116

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55	Dynamics of the Dissociation of Hydrogen on Stepped Platinum Surfaces Using the ReaxFF Reactive Force Field. Journal of Physical Chemistry B, 2006, 110, 4274-4282.	2.6	116
56	From Tree to Tape: Direct Synthesis of Pressure Sensitive Adhesives from Depolymerized Raw Lignocellulosic Biomass. ACS Central Science, 2018, 4, 701-708.	11.3	116
57	Microreactor Modeling for Hydrogen Production from Ammonia Decomposition on Ruthenium. Industrial & Engineering Chemistry Research, 2004, 43, 2986-2999.	3.7	115
58	A Review of Multiscale Analysis: Examples from Systems Biology, Materials Engineering, and Other Fluidâ€“Surface Interacting Systems. Advances in Chemical Engineering, 2005, 30, 1-61.	0.9	115
59	The chain length effect in pyrolysis: bridging the gap between glucose and cellulose. Green Chemistry, 2012, 14, 1284.	9.0	114
60	Tandem Lewis/BrÃ¸nsted homogeneous acid catalysis: conversion of glucose to 5-hydoxymethylfurfural in an aqueous chromium(<scp>iii</scp>) chloride and hydrochloric acid solution. Green Chemistry, 2015, 17, 4725-4735.	9.0	114
61	Converting fructose to 5-hydroxymethylfurfural: a quantum mechanics/molecular mechanics study of the mechanism and energetics. Carbohydrate Research, 2011, 346, 664-672.	2.3	112
62	Polypropylene Plastic Waste Conversion to Lubricants over Ru/TiO₂ Catalysts. ACS Catalysis, 2021, 11, 8104-8115.	11.2	112
63	A Theoretical and Computational Analysis of Linear Free Energy Relations for the Estimation of Activation Energies. ACS Catalysis, 2012, 2, 1624-1634.	11.2	110
64	Guaiacol Hydrodeoxygenation Mechanism on Pt(111): Insights from Density Functional Theory and Linear Free Energy Relations. ChemSusChem, 2015, 8, 315-322.	6.8	109
65	First-Principles-Based Kinetic Monte Carlo Simulation of the Structure Sensitivity of the Waterâ€“Gas Shift Reaction on Platinum Surfaces. Journal of Physical Chemistry C, 2011, 115, 24750-24762.	3.1	108
66	Coarse-grained stochastic processes and Monte Carlo simulations in lattice systems. Journal of Computational Physics, 2003, 186, 250-278.	3.8	107
67	Differentiation of Oâ€“H and Câ€“H Bond Scission Mechanisms of Ethylene Glycol on Pt and Ni/Pt Using Theory and Isotopic Labeling Experiments. Journal of the American Chemical Society, 2011, 133, 7996-8004.	13.7	107
68	Coarse-grained stochastic processes for microscopic lattice systems. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 782-787.	7.1	106
69	Fluorescence confocal optical microscopy imaging of the grain boundary structure of zeolite MFI membranes made by secondary (seeded) growth. Journal of Membrane Science, 2001, 182, 103-109.	8.2	104
70	Formation and Structure of Self-Assembled Silica Nanoparticles in Basic Solutions of Organic and Inorganic Cations. Langmuir, 2005, 21, 5197-5206.	3.5	104
71	Kinetic and Thermodynamic Studies of Silica Nanoparticle Dissolution. Chemistry of Materials, 2007, 19, 4189-4197.	6.7	104
72	Cascade of Liquidâ€Phase Catalytic Transfer Hydrogenation and Etherification of 5â€Hydroxymethylfurfural to Potential Biodiesel Components over Lewis Acid Zeolites. ChemCatChem, 2014, 6, 508-513.	3.7	104

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73	Multiscale integration hybrid algorithms for homogeneousâ€“heterogeneous reactors. AICHE Journal, 1997, 43, 3031-3041.	3.6	102
74	Dielsâ€“Alder cycloaddition of 2-methylfuran and ethylene for renewable toluene. Applied Catalysis B: Environmental, 2016, 180, 487-496.	20.2	102
75	Combined DFT, Microkinetic, and Experimental Study of Ethanol Steam Reforming on Pt. Journal of Physical Chemistry C, 2013, 117, 4691-4706.	3.1	101
76	Theoretical Approach To Predict the Stability of Supported Single-Atom Catalysts. ACS Catalysis, 2019, 9, 3289-3297.	11.2	101
77	Density Functional Theory-Derived Group Additivity and Linear Scaling Methods for Prediction of Oxygenate Stability on Metal Catalysts: Adsorption of Open-Ring Alcohol and Polyol Dehydrogenation Intermediates on Pt-Based Metals. Journal of Physical Chemistry C, 2010, 114, 20155-20166.	3.1	100
78	Pt catalysts for efficient aerobic oxidation of glucose to glucaric acid in water. Green Chemistry, 2016, 18, 3815-3822.	9.0	100
79	Fabrication of Single-Channel Catalytic Microburners:Â Effect of Confinement on the Oxidation of Hydrogen/Air Mixtures. Industrial & Engineering Chemistry Research, 2004, 43, 4833-4840.	3.7	96
80	Kinetic Regime Change in the Tandem Dehydrative Aromatization of Furan Dielsâ€“Alder Products. ACS Catalysis, 2015, 5, 2367-2375.	11.2	96
81	A C₁ microkinetic model for methane conversion to syngas on Rh/Al₂O₃. AICHE Journal, 2009, 55, 993-1008.	3.6	95
82	Correlating extent of Ptâ€“Ni bond formation with low-temperature hydrogenation of benzene and 1,3-butadiene over supported Pt/Ni bimetallic catalysts. Journal of Catalysis, 2010, 271, 239-250.	6.2	95
83	Polyethylene Hydrogenolysis at Mild Conditions over Ruthenium on Tungstated Zirconia. Jacs Au, 2021, 1, 1422-1434.	7.9	95
84	Liquidâ€Phase Catalytic Transfer Hydrogenation of Furfural over Homogeneous Lewis Acidâ€“Ru/C Catalysts. ChemSusChem, 2015, 8, 2046-2054.	6.8	93
85	Elucidating the Roles of Zeolite H-BEA in Aqueous-Phase Fructose Dehydration and HMF Rehydration. ACS Catalysis, 2013, 3, 1279-1291.	11.2	92
86	Identification of Descriptors for the CO Interaction with Metal Nanoparticles. Nano Letters, 2010, 10, 1041-1045.	9.1	91
87	The role of radical wall quenching in flame stability and wall heat flux: hydrogen-air mixtures. Combustion Theory and Modelling, 1998, 2, 515-530.	1.9	89
88	Challenges of and Insights into Acid-Catalyzed Transformations of Sugars. Journal of Physical Chemistry C, 2014, 118, 22815-22833.	3.1	88
89	Mechanistic Study of the Direct Hydrodeoxygenation of m-Cresol over WO_x-Decorated Pt/C Catalysts. ACS Catalysis, 2018, 8, 7749-7759.	11.2	87
90	Evolution of Self-Assembled Silicaâ^'Tetrapropylammonium Nanoparticles at Elevated Temperatures. Journal of Physical Chemistry B, 2005, 109, 12762-12771.	2.6	86

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91	p-Xylene Formation by Dehydrative Aromatization of a Dielsâ€“Alder Product in Lewis and BrÃ¸nsted Acidic Zeolites. Journal of Physical Chemistry C, 2014, 118, 24415-24424.	3.1	85
92	Conjugation-Driven â€œReverse Marsâ€“van Krevelenâ€•Type Radical Mechanism for Low-Temperature Câ€“O Bond Activation. Journal of the American Chemical Society, 2016, 138, 8104-8113.	13.7	84
93	Biomass-Derived Butadiene by Dehydra-Decyclization of Tetrahydrofuran. ACS Sustainable Chemistry and Engineering, 2017, 5, 3732-3736.	6.7	84
94	Fundamentals of Câ€“O bond activation on metal oxide catalysts. Nature Catalysis, 2019, 2, 269-276.	34.4	82
95	Overcoming stiffness in stochastic simulation stemming from partial equilibrium: A multiscale Monte Carlo algorithm. Journal of Chemical Physics, 2005, 123, 144114.	3.0	81
96	Recent Advances in the Photocatalytic Conversion of Biomass-Derived Furanic Compounds. ACS Catalysis, 2021, 11, 11336-11359.	11.2	81
97	Construction and optimization of complex surface-reaction mechanisms. AICHE Journal, 2000, 46, 2017-2029.	3.6	80
98	Thermal Management in Catalytic Microreactors. Industrial & Engineering Chemistry Research, 2006, 45, 76-84.	3.7	80
99	Correlating Ethylene Glycol Reforming Activity with In Situ EXAFS Detection of Ni Segregation in Supported NiPt Bimetallic Catalysts. ACS Catalysis, 2012, 2, 2290-2296.	11.2	80
100	A DFT study of furan hydrogenation and ring opening on Pd(111). Green Chemistry, 2014, 16, 736-747.	9.0	80
101	Site-Dependent Lewis Acidity of Î³-Al₂O₃ and Its Impact on Ethanol Dehydration and Etherification. Journal of Physical Chemistry C, 2014, 118, 12899-12907.	3.1	80
102	Silica Self-Assembly and Synthesis of Microporous and Mesoporous Silicates. Chemistry - A European Journal, 2006, 12, 2926-2934.	3.3	79
103	The effect of oxide acidity on HMF etherification. Catalysis Science and Technology, 2014, 4, 3074-3081.	4.1	79
104	Kinetics of faceting of crystals in growth, etching, and equilibrium. Physical Review B, 1993, 47, 4896-4909.	3.2	78
105	Infrared spectroscopy data- and physics-driven machine learning for characterizing surface microstructure of complex materials. Nature Communications, 2020, 11, 1513.	12.8	77
106	Coarse-grained stochastic processes and kinetic Monte Carlo simulators for the diffusion of interacting particles. Journal of Chemical Physics, 2003, 119, 9412-9427.	3.0	76
107	Ab initio molecular dynamics of hydrogen dissociation on metal surfaces using neural networks and novelty sampling. Journal of Chemical Physics, 2007, 127, 154716.	3.0	75
108	A Catalytic Reaction Mechanism for Methane Partial Oxidation at Short Contact Times, Reforming, and Combustion, and for Oxygenate Decomposition and Oxidation on Platinum. Industrial & Engineering Chemistry Research, 2007, 46, 5310-5324.	3.7	75

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109	Mechanistic Insights into Lewis Acid Metal Salt-Catalyzed Glucose Chemistry in Aqueous Solution. ACS Catalysis, 2016, 6, 1497-1504.	11.2	74
110	Simulations and experiments on the growth and microstructure of zeolite MFI films and membranes made by secondary growth. Microporous and Mesoporous Materials, 2001, 42, 191-203.	4.4	73
111	Kinetic Modeling of Pt Catalyzed and Computation-Driven Catalyst Discovery for Ethylene Glycol Decomposition. ACS Catalysis, 2011, 1, 1246-1256.	11.2	72
112	Solventless Câ€“C Coupling of Low Carbon Furanics to High Carbon Fuel Precursors Using an Improved Graphene Oxide Carbocatalyst. ACS Catalysis, 2017, 7, 3905-3915.	11.2	72
113	A Generalized Approach for Predicting Coverage-Dependent Reaction Parameters of Complex Surface Reactions:â€‰ Application to H2 Oxidation over Platinum. Journal of Physical Chemistry A, 1999, 103, 8101-8107.	2.5	71
114	Tungsten carbides as selective deoxygenation catalysts: experimental and computational studies of converting C3 oxygenates to propene. Green Chemistry, 2014, 16, 761-769.	9.0	71
115	Understanding solvent effects on adsorption and protonation in porous catalysts. Nature Communications, 2020, 11, 1060.	12.8	71
116	Single pot catalyst strategy to branched products via adhesive isomerization and hydrocracking of polyethylene over platinum tungstated zirconia. Applied Catalysis B: Environmental, 2021, 299, 120483.	20.2	71
117	CFD Simulations of Coupled, Countercurrent Combustor/Reformer Microdevices for Hydrogen Production. Industrial & Engineering Chemistry Research, 2005, 44, 4982-4992.	3.7	70
118	Patched bimetallic surfaces are active catalysts for ammonia decomposition. Nature Communications, 2015, 6, 8619.	12.8	70
119	Assessment of Overall Rate Expressions and Multiscale, Microkinetic Model Uniqueness via Experimental Data Injection: Ammonia Decomposition on Ru/Î³-Al₂O₃ for Hydrogen Production. Industrial & Engineering Chemistry Research, 2009, 48, 5255-5265.	3.7	69
120	Mechanism of Dehydration of Phenols on Noble Metals via First-Principles Microkinetic Modeling. ACS Catalysis, 2016, 6, 3047-3055.	11.2	69
121	Ignition and extinction of flames near surfaces: Combustion of CH4 in air. AICHE Journal, 1994, 40, 1005-1017.	3.6	68
122	Reactive Deposition of Metal Thin Films within Porous Supports from Supercritical Fluids. Chemistry of Materials, 2001, 13, 2023-2031.	6.7	68
123	BrÃ¸nstedâ€“Evansâ€“Polanyi and Transition State Scaling Relations of Furan Derivatives on Pd(111) and Their Relation to Those of Small Molecules. ACS Catalysis, 2014, 4, 604-612.	11.2	68
124	A perspective on the modeling of biomass processing. Energy and Environmental Science, 2012, 5, 6703.	30.8	66
125	Ethanol Activation on Closed-Packed Surfaces. Industrial & Engineering Chemistry Research, 2015, 54, 4213-4225.	3.7	66
126	Chemoselective Hydrodeoxygenation of Carboxylic Acids to Hydrocarbons over Nitrogen-Doped Carbonâ€“Alumina Hybrid Supported Iron Catalysts. ACS Catalysis, 2019, 9, 1564-1577.	11.2	66

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127	Insights into the isomerization of xylose to xylulose and lyxose by a Lewis acid catalyst. Carbohydrate Research, 2013, 368, 89-95.	2.3	65
128	Homogeneous Metal Salt Solutions for Biomass Upgrading and Other Select Organic Reactions. ACS Catalysis, 2019, 9, 9923-9952.	11.2	65
129	Hydrodeoxygenation of HMF over Pt/C in a continuous flow reactor. AICHE Journal, 2015, 61, 590-597.	3.6	64
130	Tunable Oleo-Furan Surfactants by Acylation of Renewable Furans. ACS Central Science, 2016, 2, 820-824.	11.3	64
131	Derivation and Validation of Mesoscopic Theories for Diffusion of Interacting Molecules. Physical Review Letters, 2000, 85, 3898-3901.	7.8	63
132	Building large microkinetic models with first-principles×3 accuracy at reduced computational cost. Chemical Engineering Science, 2015, 121, 190-199.	3.8	63
133	Deactivation of Pt/Al2O3 during propane oxidation at low temperatures: Kinetic regimes and platinum oxide formation. Journal of Catalysis, 2016, 337, 122-132.	6.2	63
134	Polyolefin plastic waste hydroconversion to fuels, lubricants, and waxes: a comparative study. Reaction Chemistry and Engineering, 2021, 7, 41-54.	3.7	61
135	Programmable heating and quenching for efficient thermochemical synthesis. Nature, 2022, 605, 470-476.	27.8	61
136	Insights into the Cr(<scp>iii</scp>) catalyzed isomerization mechanism of glucose to fructose in the presence of water using ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2014, 16, 19564-19572.	2.8	59
137	Optimization of the facet structure of transition-metal catalysts applied to the oxygen reduction reaction. Nature Chemistry, 2019, 11, 449-456.	13.6	57
138	Time accelerated Monte Carlo simulations of biological networks using the binomial Â-leap method. Bioinformatics, 2005, 21, 2136-2137.	4.1	56
139	Methane steam reforming at microscales: Operation strategies for variable power output at millisecond contact times. AICHE Journal, 2009, 55, 180-191.	3.6	56
140	Microkinetic Modeling and Reduced Rate Expressions of Ethylene Hydrogenation and Ethane Hydrogenolysis on Platinum. Industrial & Engineering Chemistry Research, 2011, 50, 28-40.	3.7	56
141	A First Principlesâ€Based Microkinetic Model for the Conversion of Fructose to 5â€Hydroxymethylfurfural. ChemCatChem, 2012, 4, 504-511.	3.7	56
142	Intensification of steam reforming of natural gas: Choosing combustible fuel and reforming catalyst. Chemical Engineering Science, 2010, 65, 398-404.	3.8	55
143	Carbohydrate dehydration using porous catalysts. Current Opinion in Chemical Engineering, 2012, 1, 312-320.	7.8	55
144	Adsorption of Acid, Ester, and Ether Functional Groups on Pt: Fast Prediction of Thermochemical Properties of Adsorbed Oxygenates via DFT-Based Group Additivity Methods. Journal of Physical Chemistry C, 2012, 116, 1873-1886.	3.1	55

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145	Adipic Acid Production via Metal-Free Selective Hydrogenolysis of Biomass-Derived Tetrahydrofuran-2,5-Dicarboxylic Acid. ACS Catalysis, 2017, 7, 6619-6634.	11.2	55
146	DFT-driven multi-site microkinetic modeling of ethanol conversion to ethylene and diethyl ether on Î³-Al2O3(1 1 1). Journal of Catalysis, 2015, 323, 121-131.	6.2	54
147	Catalytic Hydrodeoxygenation of High Carbon Furylmethanes to Renewable Jetâ€fuel Ranged Alkanes over a Rheniumâ€Modified Iridium Catalyst. ChemSusChem, 2017, 10, 3225-3234.	6.8	54
148	The Catalytic Mechanics of Dynamic Surfaces: Stimulating Methods for Promoting Catalytic Resonance. ACS Catalysis, 2020, 10, 12666-12695.	11.2	54
149	An Efficient Reaction Pathway Search Method Applied to the Decomposition of Glycerol on Platinum. Journal of Physical Chemistry C, 2011, 115, 18707-18720.	3.1	53
150	Multiscale spatial Monte Carlo simulations: Multigriding, computational singular perturbation, and hierarchical stochastic closures. Journal of Chemical Physics, 2006, 124, 064110.	3.0	52
151	Millisecond Methane Steam Reforming Via Process and Catalyst Intensification. Chemical Engineering and Technology, 2008, 31, 1201-1209.	1.5	52
152	Dominant Reaction Pathways in the Catalytic Partial Oxidation of CH4 on Rh. Topics in Catalysis, 2009, 52, 1983-1988.	2.8	52
153	Multiscale Modeling Reveals Poisoning Mechanisms of MgO-Supported Au Clusters in CO Oxidation. Nano Letters, 2012, 12, 3621-3626.	9.1	52
154	A new approach to response surface development for detailed gas-phase and surface reaction kinetic model optimization. International Journal of Chemical Kinetics, 2003, 36, 94-106.	1.6	51
155	Computational Insights into the Role of Metal and Acid Sites in Bifunctional Metal/Zeolite Catalysts: A Case Study of Acetone Hydrogenation to 2-Propanol and Subsequent Dehydration to Propene. ACS Catalysis, 2016, 6, 123-133.	11.2	51
156	The effects of phase transitions, surface diffusion, and defects on surface catalyzed reactions: Fluctuations and oscillations. Journal of Chemical Physics, 1990, 93, 8306-8313.	3.0	50
157	Parameter Optimization of Molecular Models:Â Application to Surface Kinetics. Industrial & Engineering Chemistry Research, 2003, 42, 1174-1183.	3.7	50
158	Multiscale Model and Informatics-Based Optimal Design of Experiments: Application to the Catalytic Decomposition of Ammonia on Ruthenium. Industrial & Engineering Chemistry Research, 2008, 47, 6555-6567.	3.7	50
159	Computational Insight into the Effect of Sn-Beta Na Exchange and Solvent on Glucose Isomerization and Epimerization. ACS Catalysis, 2015, 5, 5256-5263.	11.2	50
160	Reaction Pathways of Biomassâ€Derived Oxygenates over Metals and Carbides: From Model Surfaces to Supported Catalysts. ChemCatChem, 2015, 7, 1402-1421.	3.7	50
161	Insights into the Early Stages of Metal Nanoparticle Formation via First-Principle Calculations: the Roles of Citrate and Water. Langmuir, 2008, 24, 7465-7473.	3.5	49
162	Fructoseâ€“Waterâ€“Dimethylsulfoxide Interactions by Vibrational Spectroscopy and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 11274-11283.	2.6	49

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