Mark R Nimlos

List of Publications by Year
in descending order

89 papers	9,022 citations	57719 44 h-index	53190 85 g-index
91 all docs	91 docs citations	91 times ranked	9952 citing authors

#	Article	IF	Citations
1	A Conical Intersection Influences the Ground State Rearrangement of Fulvene to Benzene. Journal of Physical Chemistry A, 2022, 126, 1429-1447.	1.1	6
2	Accelerating catalyst development for biofuel production through multiscale catalytic fast pyrolysis of biomass over Mo2C. Chem Catalysis, 2022, 2, 1819-1831.	2.9	5
3	Oxidation and pyrolysis of methyl propyl ether. International Journal of Chemical Kinetics, 2021, 53, 915-938.	1.0	15
4	Efficacy, economics, and sustainability of bio-based insecticides from thermochemical biorefineries. Green Chemistry, 2021, 23, 10145-10156.	4.6	5
5	Detailed Oil Compositional Analysis Enables Evaluation of Impact of Temperature and Biomass-to-Catalyst Ratio on ex Situ Catalytic Fast Pyrolysis of Pine Vapors over ZSM-5. ACS Sustainable Chemistry and Engineering, 2020, 8, 1762-1773.	3.2	17
6	A simple method for producing bio-based anode materials for lithium-ion batteries. Green Chemistry, 2020, 22, 7093-7108.	4.6	27
7	Ga/ZSM-5 catalyst improves hydrocarbon yields and increases alkene selectivity during catalytic fast pyrolysis of biomass with co-fed hydrogen. Green Chemistry, 2020, 22, 2403-2418.	4.6	26
8	Optimization of Biomass Pyrolysis Vapor Upgrading Using a Laminar Entrained-Flow Reactor System. Energy & Fuels, 2020, 34, 6030-6040.	2.5	6
9	Valorization of aqueous waste streams from thermochemical biorefineries. Green Chemistry, 2019, 21, 4217-4230.	4.6	31
10	Hierarchically Structured CeO2 Catalyst Particles From Nanocellulose/Alginate Templates for Upgrading of Fast Pyrolysis Vapors. Frontiers in Chemistry, 2019, 7, 730.	1.8	10
11	Theoretical Determination of Size Effects in Zeolite-Catalyzed Alcohol Dehydration. Catalysts, 2019, 9, 700.	1.6	11
12	Message-passing neural networks for high-throughput polymer screening. Journal of Chemical Physics, 2019, 150, 234111.	1.2	63
13	Chemical and Structural Effects on the Rate of Xylan Hydrolysis during Dilute Acid Pretreatment of Poplar Wood. ACS Sustainable Chemistry and Engineering, 2019, 7, 4842-4850.	3.2	10
14	Fast Pyrolysis of <i>Opuntia ficus-indica</i> (Prickly Pear) and <i>Grindelia squarrosa</i> (Gumweed). Energy & Fuels, 2018, 32, 3510-3518.	2.5	8
15	Diffusion of aromatic hydrocarbons in hierarchical mesoporous H-ZSM-5 zeolite. Catalysis Today, 2018, 312, 73-81.	2.2	44
16	Catalytic Upgrading of Biomass Pyrolysis Oxygenates with Vacuum Gas Oil Using a Davison Circulating Riser Reactor. Energy & Fuels, 2018, 32, 1733-1743.	2.5	17
17	Advancing catalytic fast pyrolysis through integrated multiscale modeling and experimentation: Challenges, progress, and perspectives. Wiley Interdisciplinary Reviews: Energy and Environment, 2018, 7, e297.	1.9	30
18	Improving biomass pyrolysis economics by integrating vapor and liquid phase upgrading. Green Chemistry, 2018, 20, 567-582.	4.6	55

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19	Consideration of the Aluminum Distribution in Zeolites in Theoretical and Experimental Catalysis Research. ACS Catalysis, 2018, 8, 770-784.	5.5	161
20	Screening Fuels for Autoignition with Small-Volume Experiments and Gaussian Process Classification. Energy & Fuels, 2018, 32, 9581-9591.	2.5	8
21	Thermal Decompositions of the Lignin Model Compounds: Salicylaldehyde and Catechol. Journal of Physical Chemistry A, 2018, 122, 5911-5924.	1.1	20
22	Role of Biopolymers in the Deactivation of ZSM-5 during Catalytic Fast Pyrolysis of Biomass. ACS Sustainable Chemistry and Engineering, 2018, 6, 10030-10038.	3.2	62
23	Predictive Model for Particle Residence Time Distributions in Riser Reactors. Part 1: Model Development and Validation. ACS Sustainable Chemistry and Engineering, 2017, 5, 2847-2856.	3.2	6
24	Catalyst Residence Time Distributions in Riser Reactors for Catalytic Fast Pyrolysis. Part 2: Pilot-Scale Simulations and Operational Parameter Study. ACS Sustainable Chemistry and Engineering, 2017, 5, 2857-2866.	3.2	8
25	Deactivation of Multilayered MFI Nanosheet Zeolite during Upgrading of Biomass Pyrolysis Vapors. ACS Sustainable Chemistry and Engineering, 2017, 5, 5477-5484.	3.2	44
26	Understanding Trends in Autoignition of Biofuels: Homologous Series of Oxygenated C5 Molecules. Journal of Physical Chemistry A, 2017, 121, 5475-5486.	1.1	16
27	Estimating the Temperature Experienced by Biomass Particles during Fast Pyrolysis Using Microscopic Analysis of Biochars. Energy & Fuels, 2017, 31, 8193-8201.	2.5	9
28	Integrated Biorefining: Coproduction of Renewable Resol Biopolymer for Aqueous Stream Valorization. ACS Sustainable Chemistry and Engineering, 2017, 5, 6615-6625.	3.2	19
29	Chemicals Derived From Biomass Thermolysis and Gasification. , 2017, , 587-600.		2
30	A Quantitative Model for the Prediction of Sooting Tendency from Molecular Structure. Energy & Fuels, 2017, 31, 9983-9990.	2.5	42
31	The thermal decomposition of the benzyl radical in a heated micro-reactor. II. Pyrolysis of the tropyl radical. Journal of Chemical Physics, 2016, 145, 014305.	1.2	28
32	Furan Production from Glycoaldehyde over HZSM-5. ACS Sustainable Chemistry and Engineering, 2016, 4, 2615-2623.	3.2	19
33	Influence of Crystal Allomorph and Crystallinity on the Products and Behavior of Cellulose during Fast Pyrolysis. ACS Sustainable Chemistry and Engineering, 2016, 4, 4662-4674.	3.2	69
34	Supported molybdenum oxides as effective catalysts for the catalytic fast pyrolysis of lignocellulosic biomass. Green Chemistry, 2016, 18, 5548-5557.	4.6	76
35	In Situ and ex Situ Catalytic Pyrolysis of Pine in a Bench-Scale Fluidized Bed Reactor System. Energy & Fuels, 2016, 30, 2144-2157.	2.5	100
36	Elucidating Zeolite Deactivation Mechanisms During Biomass Catalytic Fast Pyrolysis from Model Reactions and Zeolite Syntheses. Topics in Catalysis, 2016, 59, 73-85.	1.3	19

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37	Pyrolysis Mechanisms of Lignin Model Compounds Using a Heated Micro-Reactor. Green Chemistry and Sustainable Technology, 2016, , 145-171.	0.4	6
38	Catalytic Pyrolysis of Pine Over HZSM-5 with Different Binders. Topics in Catalysis, 2016, 59, 94-108.	1.3	32
39	Catalytic fast pyrolysis of biomass: the reactions of water and aromatic intermediates produces phenols. Green Chemistry, 2015, 17, 4217-4227.	4.6	71
40	Pyrolysis of Cyclopentadienone: Mechanistic Insights from a Direct Measurement of Product Branching Ratios. Journal of Physical Chemistry A, 2015, 119, 7222-7234.	1.1	23
41	Biomass Particle Models with Realistic Morphology and Resolved Microstructure for Simulations of Intraparticle Transport Phenomena. Energy & Fuels, 2015, 29, 242-254.	2.5	66
42	Molybdenum incorporated mesoporous silica catalyst for production of biofuels and value-added chemicals via catalytic fast pyrolysis. Green Chemistry, 2015, 17, 3035-3046.	4.6	45
43	Ethanol Dehydration in HZSM-5 Studied by Density Functional Theory: Evidence for a Concerted Process. Journal of Physical Chemistry A, 2015, 119, 3604-3614.	1.1	44
44	Carbocation Stability in H-ZSM5 at High Temperature. Journal of Physical Chemistry A, 2015, 119, 11397-11405.	1.1	14
45	The thermal decomposition of the benzyl radical in a heated micro-reactor. I. Experimental findings. Journal of Chemical Physics, 2015, 142, 044307.	1.2	46
46	Upgrading biomass pyrolysis vapors over Î²-zeolites: role of silica-to-alumina ratio. Green Chemistry, 2014, 16, 4891-4905.	4.6	91
47	Polarized Matrix Infrared Spectra of Cyclopentadienone: Observations, Calculations, and Assignment for an Important Intermediate in Combustion and Biomass Pyrolysis. Journal of Physical Chemistry A, 2014, 118, 708-718.	1.1	27
48	Unimolecular thermal decomposition of dimethoxybenzenes. Journal of Chemical Physics, 2014, 140, 234302.	1.2	30
49	Real-time monitoring of the deactivation of HZSM-5 during upgrading of pine pyrolysis vapors. Green Chemistry, 2014, 16, 1444-1461.	4.6	112
50	Chirped-Pulse Fourier Transform Microwave Spectroscopy Coupled with a Flash Pyrolysis Microreactor: Structural Determination of the Reactive Intermediate Cyclopentadienone. Journal of Physical Chemistry Letters, 2014, 5, 2201-2207.	2.1	27
51	A Mechanistic Investigation of Acid-Catalyzed Cleavage of Aryl-Ether Linkages: Implications for Lignin Depolymerization in Acidic Environments. ACS Sustainable Chemistry and Engineering, 2014, 2, 472-485.	3.2	317
52	A perspective on oxygenated species in the refinery integration of pyrolysis oil. Green Chemistry, 2014, 16, 407-453.	4.6	235
53	Investigation of Xylose Reversion Reactions That Can Occur during Dilute Acid Pretreatment. Energy & Fuels, 2013, 27, 7389-7397.	2.5	5
54	Pyrolysis of furan in a microreactor. Journal of Chemical Physics, 2013, 139, 124305.	1.2	63

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55	Biomass pyrolysis: Thermal decomposition mechanisms of furfural and benzaldehyde. Journal of Chemical Physics, 2013, 139, 104310.	1.2	63
56	Thermal decomposition of CH3CHO studied by matrix infrared spectroscopy and photoionization mass spectroscopy. Journal of Chemical Physics, 2012, 137, 164308.	1.2	49
57	Unimolecular thermal decomposition of phenol and d5-phenol: Direct observation of cyclopentadiene formation via cyclohexadienone. Journal of Chemical Physics, 2012, 136, 044309.	1.2	64
58	Binding Preferences, Surface Attachment, Diffusivity, and Orientation of a Family 1 Carbohydrate-binding Module on Cellulose. Journal of Biological Chemistry, 2012, 287, 20603-20612.	1.6	76
59	Direct Detection of Products from the Pyrolysis of 2-Phenethyl Phenyl Ether. Journal of Physical Chemistry A, 2011, 115, 428-438.	1.1	160
60	Thermal Decomposition Mechanisms of the Methoxyphenols: Formation of Phenol, Cyclopentadienone, Vinylacetylene, and Acetylene. Journal of Physical Chemistry A, 2011, 115, 13381-13389.	1.1	80
61	Computational Study of Bond Dissociation Enthalpies for a Large Range of Native and Modified Lignins. Journal of Physical Chemistry Letters, 2011, 2, 2846-2852.	2.1	318
62	Elucidation of Biomass Pyrolysis Products Using a Laminar Entrained Flow Reactor and Char Particle Imaging. Energy & Fuels, 2011, 25, 324-336.	2.5	61
63	Biomass Pyrolysis and Gasification of Varying Particle Sizes in a Fluidized-Bed Reactor. Energy & Fuels, 2011, 25, 3747-3757.	2.5	73
64	Laser ablation with resonance-enhanced multiphoton ionization time-of-flight mass spectrometry for determining aromatic lignin volatilization products from biomass. Review of Scientific Instruments, 2011, 82, 033104.	0.6	37
65	Probing Carbohydrate Product Expulsion from a Processive Cellulase with Multiple Absolute Binding Free Energy Methods. Journal of Biological Chemistry, 2011, 286, 18161-18169.	1.6	69
66	Pilot-Scale Gasification of Corn Stover, Switchgrass, Wheat Straw, and Wood: 1. Parametric Study and Comparison with Literature. Industrial & Engineering Chemistry Research, 2010, 49, 1859-1871.	1.8	136
67	Meso-Scale Modeling of Polysaccharides in Plant Cell Walls: An Application to Translation of CBMs on the Cellulose Surface. ACS Symposium Series, 2010, , 99-117.	0.5	3
68	Radical Chemistry in the Thermal Decomposition of Anisole and Deuterated Anisoles: An Investigation of Aromatic Growth. Journal of Physical Chemistry A, 2010, 114, 9043-9056.	1.1	96
69	Glucose Reversion Reaction Kinetics. Journal of Agricultural and Food Chemistry, 2010, 58, 6131-6140.	2.4	84
70	Identification of Amino Acids Responsible for Processivity in a Family 1 Carbohydrate-Binding Module from a Fungal Cellulase. Journal of Physical Chemistry B, 2010, 114, 1447-1453.	1.2	116
71	Pilot-Scale Gasification of Corn Stover, Switchgrass, Wheat Straw, and Wood: 2. Identification of Global Chemistry Using Multivariate Curve Resolution Techniques. Industrial & Engineering Chemistry Research, 2009, 48, 10691-10701.	1.8	30
72	The Energy Landscape for the Interaction of the Family 1 Carbohydrate-Binding Module and the Cellulose Surface is Altered by Hydrolyzed Glycosidic Bonds. Journal of Physical Chemistry B, 2009, 113, 10994-11002.	1.2	75

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73	Interactions of the complete cellobiohydrolase I from Trichodera reesei with microcrystalline cellulose Iî². Cellulose, 2008, 15, 261-273.	2.4	46
74	Calculated Hydride Donor Abilities of Five-Coordinate Transition Metal Hydrides [HM(diphosphine)₂]⁺ (M = Ni, Pd, Pt) as a Function of the Bite Angle and Twist Angle of Diphosphine Ligands. Organometallics, 2008, 27, 2715-2722.	1.1	65
75	Molecular modeling suggests induced fit of Family I carbohydrate-binding modules with a broken-chain cellulose surface. Protein Engineering, Design and Selection, 2007, 20, 179-187.	1.0	79
76	Unimolecular thermal fragmentation ofortho-benzyne. Journal of Chemical Physics, 2007, 126, 044312.	1.2	73
77	Biomass Recalcitrance: Engineering Plants and Enzymes for Biofuels Production. Science, 2007, 315, 804-807.	6.0	3,749
78	Energetics of Xylose Decomposition as Determined Using Quantum Mechanics Modeling. Journal of Physical Chemistry A, 2006, 110, 11824-11838.	1.1	140
79	Mechanisms of Glycerol Dehydration. Journal of Physical Chemistry A, 2006, 110, 6145-6156.	1.1	239
80	Ab initio molecular dynamics simulations of î²-d-glucose and î²-d-xylose degradation mechanisms in acidic aqueous solution. Carbohydrate Research, 2005, 340, 2319-2327.	1.1	142
81	Hydrogen Atom Mediated Stoneâ˘'Wales Rearrangement of Pyracyclene:â€‰ A Model for Annealing in Fullerene Formation. Journal of Physical Chemistry A, 2005, 109, 9896-9903.	1.1	24
82	Acidic Sugar Degradation Pathways. , 2005, , 989-997.		5
83	Intense, hyperthermal source of organic radicals for matrix-isolation spectroscopy. Review of Scientific Instruments, 2003, 74, 3077-3086.	0.6	83
84	A study of the mechanisms of vanillin pyrolysis by mass spectrometry and multivariate analysis. Fuel, 2001, 80, 1689-1696.	3.4	67
85	Kinetic analysis of the gas-phase pyrolysis of carbohydrates. Fuel, 2001, 80, 1697-1709.	3.4	101
86	The pyrolysis of anisole (C6H5OCH3) using a hyperthermal nozzle. Fuel, 2001, 80, 1747-1755.	3.4	84
87	Gas-Phase Heterogeneous Photocatalytic Oxidation of Ethanol:Â Pathways and Kinetic Modeling. Environmental Science & Technology, 1996, 30, 3102-3110.	4.6	175
88	Mechanisms of Xylose and Xylo-Oligomer Degradation During Acid Pretreatment. , 0, , 331-351.		4
89	Multiscale Catalytic Fast Pyrolysis of Grindelia Reveals Opportunities for Generating Low Oxygen Content Bio-Oils from Drought Tolerant Biomass. Energy & Fuels, 0, , .	2.5	0