Mark R Nimlos

List of Publications by Year
in descending order

89 papers	9,022 citations	57758 44 h-index	53230 85 g-index
91 all docs	91 docs citations	91 times ranked	9952 citing authors

#	Article	IF	Citations
1	Biomass Recalcitrance: Engineering Plants and Enzymes for Biofuels Production. Science, 2007, 315, 804-807.	12.6	3,749
2	Computational Study of Bond Dissociation Enthalpies for a Large Range of Native and Modified Lignins. Journal of Physical Chemistry Letters, 2011, 2, 2846-2852.	4.6	318
3	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.	6.7	317
4	Mechanisms of Glycerol Dehydration. Journal of Physical Chemistry A, 2006, 110, 6145-6156.	2.5	239
5	A perspective on oxygenated species in the refinery integration of pyrolysis oil. Green Chemistry, 2014, 16, 407-453.	9.0	235
6	Gas-Phase Heterogeneous Photocatalytic Oxidation of Ethanol:Â Pathways and Kinetic Modeling. Environmental Science & Technology, 1996, 30, 3102-3110.	10.0	175
7	Consideration of the Aluminum Distribution in Zeolites in Theoretical and Experimental Catalysis Research. ACS Catalysis, 2018, 8, 770-784.	11.2	161
8	Direct Detection of Products from the Pyrolysis of 2-Phenethyl Phenyl Ether. Journal of Physical Chemistry A, 2011, 115, 428-438.	2.5	160
9	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.	2.3	142
10	Energetics of Xylose Decomposition as Determined Using Quantum Mechanics Modeling. Journal of Physical Chemistry A, 2006, 110, 11824-11838.	2.5	140
11	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.	3.7	136
12	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.	2.6	116
13	Real-time monitoring of the deactivation of HZSM-5 during upgrading of pine pyrolysis vapors. Green Chemistry, 2014, 16, 1444-1461.	9.0	112
14	Kinetic analysis of the gas-phase pyrolysis of carbohydrates. Fuel, 2001, 80, 1697-1709.	6.4	101
15	In Situ and ex Situ Catalytic Pyrolysis of Pine in a Bench-Scale Fluidized Bed Reactor System. Energy & Fuels, 2016, 30, 2144-2157.	5.1	100
16	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.	2.5	96
17	Upgrading biomass pyrolysis vapors over Î²-zeolites: role of silica-to-alumina ratio. Green Chemistry, 2014, 16, 4891-4905.	9.0	91
18	The pyrolysis of anisole (C6H5OCH3) using a hyperthermal nozzle. Fuel, 2001, 80, 1747-1755.	6.4	84

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19	Glucose Reversion Reaction Kinetics. Journal of Agricultural and Food Chemistry, 2010, 58, 6131-6140.	5.2	84
20	Intense, hyperthermal source of organic radicals for matrix-isolation spectroscopy. Review of Scientific Instruments, 2003, 74, 3077-3086.	1.3	83
21	Thermal Decomposition Mechanisms of the Methoxyphenols: Formation of Phenol, Cyclopentadienone, Vinylacetylene, and Acetylene. Journal of Physical Chemistry A, 2011, 115, 13381-13389.	2.5	80
22	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.	2.1	79
23	Binding Preferences, Surface Attachment, Diffusivity, and Orientation of a Family 1 Carbohydrate-binding Module on Cellulose. Journal of Biological Chemistry, 2012, 287, 20603-20612.	3.4	76
24	Supported molybdenum oxides as effective catalysts for the catalytic fast pyrolysis of lignocellulosic biomass. Green Chemistry, 2016, 18, 5548-5557.	9.0	76
25	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.	2.6	75
26	Unimolecular thermal fragmentation ofortho-benzyne. Journal of Chemical Physics, 2007, 126, 044312.	3.0	73
27	Biomass Pyrolysis and Gasification of Varying Particle Sizes in a Fluidized-Bed Reactor. Energy & Fuels, 2011, 25, 3747-3757.	5.1	73
28	Catalytic fast pyrolysis of biomass: the reactions of water and aromatic intermediates produces phenols. Green Chemistry, 2015, 17, 4217-4227.	9.0	71
29	Probing Carbohydrate Product Expulsion from a Processive Cellulase with Multiple Absolute Binding Free Energy Methods. Journal of Biological Chemistry, 2011, 286, 18161-18169.	3.4	69
30	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.	6.7	69
31	A study of the mechanisms of vanillin pyrolysis by mass spectrometry and multivariate analysis. Fuel, 2001, 80, 1689-1696.	6.4	67
32	Biomass Particle Models with Realistic Morphology and Resolved Microstructure for Simulations of Intraparticle Transport Phenomena. Energy & Fuels, 2015, 29, 242-254.	5.1	66
33	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.	2.3	65
34	Unimolecular thermal decomposition of phenol and d5-phenol: Direct observation of cyclopentadiene formation via cyclohexadienone. Journal of Chemical Physics, 2012, 136, 044309.	3.0	64
35	Pyrolysis of furan in a microreactor. Journal of Chemical Physics, 2013, 139, 124305.	3.0	63
36	Biomass pyrolysis: Thermal decomposition mechanisms of furfural and benzaldehyde. Journal of Chemical Physics, 2013, 139, 104310.	3.0	63

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37	Message-passing neural networks for high-throughput polymer screening. Journal of Chemical Physics, 2019, 150, 234111.	3.0	63
38	Role of Biopolymers in the Deactivation of ZSM-5 during Catalytic Fast Pyrolysis of Biomass. ACS Sustainable Chemistry and Engineering, 2018, 6, 10030-10038.	6.7	62
39	Elucidation of Biomass Pyrolysis Products Using a Laminar Entrained Flow Reactor and Char Particle Imaging. Energy & Fuels, 2011, 25, 324-336.	5.1	61
40	Improving biomass pyrolysis economics by integrating vapor and liquid phase upgrading. Green Chemistry, 2018, 20, 567-582.	9.0	55
41	Thermal decomposition of CH3CHO studied by matrix infrared spectroscopy and photoionization mass spectroscopy. Journal of Chemical Physics, 2012, 137, 164308.	3.0	49
42	Interactions of the complete cellobiohydrolase I from Trichodera reesei with microcrystalline cellulose Iβ. Cellulose, 2008, 15, 261-273.	4.9	46
43	The thermal decomposition of the benzyl radical in a heated micro-reactor. I. Experimental findings. Journal of Chemical Physics, 2015, 142, 044307.	3.0	46
44	Molybdenum incorporated mesoporous silica catalyst for production of biofuels and value-added chemicals via catalytic fast pyrolysis. Green Chemistry, 2015, 17, 3035-3046.	9.0	45
45	Ethanol Dehydration in HZSM-5 Studied by Density Functional Theory: Evidence for a Concerted Process. Journal of Physical Chemistry A, 2015, 119, 3604-3614.	2.5	44
46	Deactivation of Multilayered MFI Nanosheet Zeolite during Upgrading of Biomass Pyrolysis Vapors. ACS Sustainable Chemistry and Engineering, 2017, 5, 5477-5484.	6.7	44
47	Diffusion of aromatic hydrocarbons in hierarchical mesoporous H-ZSM-5 zeolite. Catalysis Today, 2018, 312, 73-81.	4.4	44
48	A Quantitative Model for the Prediction of Sooting Tendency from Molecular Structure. Energy & Fuels, 2017, 31, 9983-9990.	5.1	42
49	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.	1.3	37
50	Catalytic Pyrolysis of Pine Over HZSM-5 with Different Binders. Topics in Catalysis, 2016, 59, 94-108.	2.8	32
51	Valorization of aqueous waste streams from thermochemical biorefineries. Green Chemistry, 2019, 21, 4217-4230.	9.0	31
52	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.	3.7	30
53	Unimolecular thermal decomposition of dimethoxybenzenes. Journal of Chemical Physics, 2014, 140, 234302.	3.0	30
54	Advancing catalytic fast pyrolysis through integrated multiscale modeling and experimentation: Challenges, progress, and perspectives. Wiley Interdisciplinary Reviews: Energy and Environment, 2018, 7, e297.	4.1	30

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55	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.	3.0	28
56	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.	2.5	27
57	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.	4.6	27
58	A simple method for producing bio-based anode materials for lithium-ion batteries. Green Chemistry, 2020, 22, 7093-7108.	9.0	27
59	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.	9.0	26
60	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.	2.5	24
61	Pyrolysis of Cyclopentadienone: Mechanistic Insights from a Direct Measurement of Product Branching Ratios. Journal of Physical Chemistry A, 2015, 119, 7222-7234.	2.5	23
62	Thermal Decompositions of the Lignin Model Compounds: Salicylaldehyde and Catechol. Journal of Physical Chemistry A, 2018, 122, 5911-5924.	2.5	20
63	Furan Production from Glycoaldehyde over HZSM-5. ACS Sustainable Chemistry and Engineering, 2016, 4, 2615-2623.	6.7	19
64	Elucidating Zeolite Deactivation Mechanisms During Biomass Catalytic Fast Pyrolysis from Model Reactions and Zeolite Syntheses. Topics in Catalysis, 2016, 59, 73-85.	2.8	19
65	Integrated Biorefining: Coproduction of Renewable Resol Biopolymer for Aqueous Stream Valorization. ACS Sustainable Chemistry and Engineering, 2017, 5, 6615-6625.	6.7	19
66	Catalytic Upgrading of Biomass Pyrolysis Oxygenates with Vacuum Gas Oil Using a Davison Circulating Riser Reactor. Energy & Fuels, 2018, 32, 1733-1743.	5.1	17
67	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.	6.7	17
68	Understanding Trends in Autoignition of Biofuels: Homologous Series of Oxygenated C5 Molecules. Journal of Physical Chemistry A, 2017, 121, 5475-5486.	2.5	16
69	Oxidation and pyrolysis of methyl propyl ether. International Journal of Chemical Kinetics, 2021, 53, 915-938.	1.6	15
70	Carbocation Stability in H-ZSM5 at High Temperature. Journal of Physical Chemistry A, 2015, 119, 11397-11405.	2.5	14
71	Theoretical Determination of Size Effects in Zeolite-Catalyzed Alcohol Dehydration. Catalysts, 2019, 9, 700.	3.5	11
72	Hierarchically Structured CeO2 Catalyst Particles From Nanocellulose/Alginate Templates for Upgrading of Fast Pyrolysis Vapors. Frontiers in Chemistry, 2019, 7, 730.	3.6	10

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73	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.	6.7	10
74	Estimating the Temperature Experienced by Biomass Particles during Fast Pyrolysis Using Microscopic Analysis of Biochars. Energy & Fuels, 2017, 31, 8193-8201.	5.1	9
75	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.	6.7	8
76	Fast Pyrolysis of <i>Opuntia ficus-indica</i> (Prickly Pear) and <i>Grindelia squarrosa</i> (Gumweed). Energy & Fuels, 2018, 32, 3510-3518.	5.1	8
77	Screening Fuels for Autoignition with Small-Volume Experiments and Gaussian Process Classification. Energy & Fuels, 2018, 32, 9581-9591.	5.1	8
78	Pyrolysis Mechanisms of Lignin Model Compounds Using a Heated Micro-Reactor. Green Chemistry and Sustainable Technology, 2016, , 145-171.	0.7	6
79	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.	6.7	6
80	Optimization of Biomass Pyrolysis Vapor Upgrading Using a Laminar Entrained-Flow Reactor System. Energy & Fuels, 2020, 34, 6030-6040.	5.1	6
81	A Conical Intersection Influences the Ground State Rearrangement of Fulvene to Benzene. Journal of Physical Chemistry A, 2022, 126, 1429-1447.	2.5	6
82	Investigation of Xylose Reversion Reactions That Can Occur during Dilute Acid Pretreatment. Energy & Fuels, 2013, 27, 7389-7397.	5.1	5
83	Acidic Sugar Degradation Pathways. , 2005, , 989-997.		5
84	Efficacy, economics, and sustainability of bio-based insecticides from thermochemical biorefineries. Green Chemistry, 2021, 23, 10145-10156.	9.0	5
85	Accelerating catalyst development for biofuel production through multiscale catalytic fast pyrolysis of biomass over Mo2C. Chem Catalysis, 2022, 2, 1819-1831.	6.1	5
86	Mechanisms of Xylose and Xylo-Oligomer Degradation During Acid Pretreatment. , 0, , 331-351.		4
87	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
88	Chemicals Derived From Biomass Thermolysis and Gasification. , 2017, , 587-600.		2
89	Multiscale Catalytic Fast Pyrolysis of Grindelia Reveals Opportunities for Generating Low Oxygen Content Bio-Oils from Drought Tolerant Biomass. Energy & Fuels, 0, , .	5.1	0