Dionisios G Vlachos

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433 papers	20,527 citations	78 h-index	122 g-index
464 ext. papers	23,162 ext. citations	7.9 avg, IF	7.42 L-index

#	Paper	IF	Citations
433	Microstructural optimization of a zeolite membrane for organic vapor separation. *Science*, **2003**, 300, 456-60	33.3	863
432	Insights into the interplay of Lewis and Brønsted 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	16.4	496
431	Top ten fundamental challenges of biomass pyrolysis for biofuels. *Energy and Environmental Science* , **2012**, 5, 7797	35.4	384
430	Mechanistic Insights into the Electrochemical Reduction of CO2 to CO on Nanostructured Ag Surfaces. *ACS Catalysis*, **2015**, 5, 4293-4299	13.1	353
429	Cycloaddition of Biomass-Derived Furans for Catalytic Production of Renewable p-Xylene. *ACS Catalysis*, **2012**, 2, 935-939	13.1	335
428	An overview of spatial microscopic and accelerated kinetic Monte Carlo methods. *Journal of Computer-Aided Materials Design*, **2007**, 14, 253-308		328
427	Using first principles to predict bimetallic catalysts for the ammonia decomposition reaction. *Nature Chemistry*, **2010**, 2, 484-9	17.6	314
426	Xylose Isomerization to Xylulose and its Dehydration to Furfural in Aqueous Media. *ACS Catalysis*, **2011**, 1, 1724-1728	13.1	271
425	Nickel supported on nitrogen-doped carbon nanotubes as hydrogen oxidation reaction catalyst in alkaline electrolyte. *Nature Communications*, **2016**, 7, 10141	17.4	269
424	Conversion of Xylose to Furfural Using Lewis and Brønsted Acid Catalysts in Aqueous Media. *ACS Catalysis*, **2012**, 2, 2022-2028	13.1	261
423	A review on microcombustion: Fundamentals, devices and applications. *Progress in Energy and Combustion Science*, **2012**, 38, 321-359	33.6	253
422	Revealing pyrolysis chemistry for biofuels production: Conversion of cellulose to furans and small oxygenates. *Energy and Environmental Science*, **2012**, 5, 5414-5424	35.4	230
421	Correlating particle size and shape of supported Ru/gamma-Al2O3 catalysts with NH3 decomposition activity. *Journal of the American Chemical Society*, **2009**, 131, 12230-9	16.4	218
420	Production of dimethylfuran from hydroxymethylfurfural through catalytic transfer hydrogenation with ruthenium supported on carbon. *ChemSusChem*, **2013**, 6, 1158-62	8.3	213
419	Molecular structure, morphology and growth mechanisms and rates of 5-hydroxymethyl furfural (HMF) derived humins. *Green Chemistry*, **2016**, 18, 1983-1993	10	201
418	Steam and dry reforming of methane on Rh: Microkinetic analysis and hierarchy of kinetic models. *Journal of Catalysis*, **2008**, 259, 211-222	7.3	192
417	DFT Study of Furfural Conversion to Furan, Furfuryl Alcohol, and 2-Methylfuran on Pd(111). *ACS Catalysis*, **2012**, 2, 2496-2504	13.1	184

416	Liquid phase catalytic transfer hydrogenation of furfural over a Ru/C catalyst. *Applied Catalysis A: General*, **2014**, 480, 17-24	5.1	180
415	Mechanistic Insights into Metal Lewis Acid-Mediated Catalytic Transfer Hydrogenation of Furfural to 2-Methylfuran. *ACS Catalysis*, **2015**, 5, 3988-3994	13.1	176
414	Zeolite Growth by Addition of Subcolloidal Particles: Modeling and Experimental Validation. *Chemistry of Materials*, **2000**, 12, 845-853	9.6	171
413	Mechanistic Study of Alcohol Dehydration on Al2O3. *ACS Catalysis*, **2012**, 2, 1846-1853	13.1	167
412	Unraveling the Complexity of Catalytic Reactions via Kinetic Monte Carlo Simulation: Current Status and Frontiers. *ACS Catalysis*, **2012**, 2, 2648-2663	13.1	158
411	Binomial distribution based tau-leap accelerated stochastic simulation. *Journal of Chemical Physics*, **2005**, 122, 024112	3.9	157
410	Structure of the Silica Phase Extracted from Silica/(TPA)OH Solutions Containing Nanoparticles. *Journal of Physical Chemistry B*, **2003**, 107, 10006-10016	3.4	153
409	Selective hydrodeoxygenation of biomass-derived oxygenates to unsaturated hydrocarbons using molybdenum carbide catalysts. *ChemSusChem*, **2013**, 6, 798-801	8.3	148
408	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		146
407	Zeolite (MFI) Crystal Morphology Control Using Organic Structure-Directing Agents. *Chemistry of Materials*, **2004**, 16, 5697-5705	9.6	145
406	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	9.6	142
405	Coverage-Induced Conformational Effects on Activity and Selectivity: Hydrogenation and Decarbonylation of Furfural on Pd(111). *ACS Catalysis*, **2015**, 5, 104-112	13.1	133
404	A graph-theoretical kinetic Monte Carlo framework for on-lattice chemical kinetics. *Journal of Chemical Physics*, **2011**, 134, 214115	3.9	133
403	Spontaneous Formation of Silica Nanoparticles in Basic Solutions of Small Tetraalkylammonium Cations. *Journal of Physical Chemistry B*, **2004**, 108, 12271-12275	3.4	130
402	DFT Study of the Water Gas Shift Reaction and Coke Formation on Ni(111) and Ni(211) Surfaces. *Journal of Physical Chemistry C*, **2012**, 116, 20281-20291	3.8	128
401	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	3.8	128
400	Thermodynamic Consistency in Microkinetic Development of Surface Reaction Mechanisms. *Journal of Physical Chemistry B*, **2003**, 107, 12721-12733	3.4	124
399	Stability and performance of catalytic microreactors: Simulations of propane catalytic combustion on Pt. *Chemical Engineering Science*, **2008**, 63, 1098-1116	4.4	123

398	Understanding solvent effects in the selective conversion of fructose to 5-hydroxymethyl-furfural: a molecular dynamics investigation. *Physical Chemistry Chemical Physics*, **2012**, 14, 2637-44	3.6	122
397	Physical basis for the formation and stability of silica nanoparticles in basic solutions of monovalent cations. *Langmuir*, **2005**, 21, 8960-71	4	116
396	Microkinetic Modeling for Water-Promoted CO Oxidation, Water Gas Shift, and Preferential Oxidation of CO on Pt. *Journal of Physical Chemistry B*, **2004**, 108, 15246-15258	3.4	115
395	A DFT study of the acid-catalyzed conversion of 2,5-dimethylfuran and ethylene to p-xylene. *Journal of Catalysis*, **2013**, 297, 35-43	7.3	114
394	Comparison of homogeneous and heterogeneous catalysts for glucose-to-fructose isomerization in aqueous media. *ChemSusChem*, **2013**, 6, 2369-76	8.3	112
393	Role of Silanol Group in Sn-Beta Zeolite for Glucose Isomerization and Epimerization Reactions. *ACS Catalysis*, **2013**, 3, 2294-2298	13.1	111
392	The Role of Ru and RuO2 in the Catalytic Transfer Hydrogenation of 5-Hydroxymethylfurfural for the Production of 2,5-Dimethylfuran. *ChemCatChem*, **2014**, 6, 848-856	5.2	111
391	Vapor phase hydrodeoxygenation of furfural to 2-methylfuran on molybdenum carbide catalysts. *Catalysis Science and Technology*, **2014**, 4, 2340	5.5	110
390	Dynamics of the dissociation of hydrogen on stepped platinum surfaces using the ReaxFF reactive force field. *Journal of Physical Chemistry B*, **2006**, 110, 4274-82	3.4	110
389	Tandem Lewis acid/Brønsted acid-catalyzed conversion of carbohydrates to 5-hydroxymethylfurfural using zeolite beta. *Journal of Catalysis*, **2016**, 333, 149-161	7.3	108
388	Density Functional Theory-Computed Mechanisms of Ethylene and Diethyl Ether Formation from Ethanol on γ-Al2O3(100). *ACS Catalysis*, **2013**, 3, 1965-1975	13.1	107
387	Mechanism of Brønsted acid-catalyzed glucose dehydration. *ChemSusChem*, **2015**, 8, 1334-41	8.3	107
386	Pyrolytic conversion of cellulose to fuels: levoglucosan deoxygenation via elimination and cyclization within molten biomass. *Energy and Environmental Science*, **2012**, 5, 7864	35.4	105
385	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, 16819-35	3.4	102
384	Differentiation of O-H and C-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	16.4	101
383	Formation and structure of self-assembled silica nanoparticles in basic solutions of organic and inorganic cations. *Langmuir*, **2005**, 21, 5197-206	4	101
382	A Review of Multiscale Analysis: Examples from Systems Biology, Materials Engineering, and Other Fluid-Surface Interacting Systems. *Advances in Chemical Engineering*, **2005**, 30, 1-61	0.6	100
381	Mechanisms for High Selectivity in the Hydrodeoxygenation of 5-Hydroxymethylfurfural over PtCo Nanocrystals. *ACS Catalysis*, **2016**, 6, 4095-4104	13.1	100

380	Effects of correlated parameters and uncertainty in electronic-structure-based chemical kinetic modelling. *Nature Chemistry*, **2016**, 8, 331-7	17.6	99
379	First-Principles-Based Kinetic Monte Carlo Simulation of the Structure Sensitivity of the Water□Gas Shift Reaction on Platinum Surfaces. *Journal of Physical Chemistry C*, **2011**, 115, 24750-24762	3.8	97
378	Coarse-grained stochastic processes for microscopic lattice systems. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 782-7	11.5	97
377	Converting fructose to 5-hydroxymethylfurfural: a quantum mechanics/molecular mechanics study of the mechanism and energetics. *Carbohydrate Research*, **2011**, 346, 664-72	2.9	95
376	Microreactor Modeling for Hydrogen Production from Ammonia Decomposition on Ruthenium. *Industrial & Engineering Chemistry Research*, **2004**, 43, 2986-2999	3.9	95
375	Kinetic and Thermodynamic Studies of Silica Nanoparticle Dissolution. *Chemistry of Materials*, **2007**, 19, 4189-4197	9.6	94
374	The chain length effect in pyrolysis: bridging the gap between glucose and cellulose. *Green Chemistry*, **2012**, 14, 1284	10	93
373	Coarse-grained stochastic processes and Monte Carlo simulations in lattice systems. *Journal of Computational Physics*, **2003**, 186, 250-278	4.1	93
372	Guaiacol hydrodeoxygenation mechanism on Pt(111): insights from density functional theory and linear free energy relations. *ChemSusChem*, **2015**, 8, 315-22	8.3	91
371	Kinetics of Homogeneous Br□sted Acid Catalyzed Fructose Dehydration and 5-Hydroxymethyl Furfural Rehydration: A Combined Experimental and Computational Study. *ACS Catalysis*, **2014**, 4, 259-267	12.1	90
370	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	3.8	90
369	Multiscale integration hybrid algorithms for homogeneous□heterogeneous reactors. *AICHE Journal*, **1997**, 43, 3031-3041	3.6	90
368	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	9.6	90
367	Tandem Lewis/Br□sted homogeneous acid catalysis: conversion of glucose to 5-hydoxymethylfurfural in an aqueous chromium(III) chloride and hydrochloric acid solution. *Green Chemistry*, **2015**, 17, 4725-4735	10	89
366	Fabrication of Single-Channel Catalytic Microburners:□Effect of Confinement on the Oxidation of Hydrogen/Air Mixtures. *Industrial & Engineering Chemistry Research*, **2004**, 43, 4833-4840	3.9	89
365	Correlating extent of Pt□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	7.3	87
364	Structural analysis of humins formed in the Br□sted acid catalyzed dehydration of fructose. *Green Chemistry*, **2018**, 20, 997-1006	10	85
363	Cascade of Liquid-Phase Catalytic Transfer Hydrogenation and Etherification of 5-Hydroxymethylfurfural to Potential Biodiesel Components over Lewis Acid Zeolites. *ChemCatChem*, **2014**, 6, 508-513	5.2	85

362	A C1 microkinetic model for methane conversion to syngas on Rh/Al2O3. *AICHE Journal*, **2009**, 55, 993-1008	3.8	83
361	Combined DFT, Microkinetic, and Experimental Study of Ethanol Steam Reforming on Pt. *Journal of Physical Chemistry C*, **2013**, 117, 4691-4706	3.8	80
360	A Theoretical and Computational Analysis of Linear Free Energy Relations for the Estimation of Activation Energies. *ACS Catalysis*, **2012**, 2, 1624-1634	13.1	80
359	Elucidating the Roles of Zeolite H-BEA in Aqueous-Phase Fructose Dehydration and HMF Rehydration. *ACS Catalysis*, **2013**, 3, 1279-1291	13.1	80
358	Evolution of self-assembled silica-tetrapropylammonium nanoparticles at elevated temperatures. *Journal of Physical Chemistry B*, **2005**, 109, 12762-71	3.4	80
357	Challenges of and Insights into Acid-Catalyzed Transformations of Sugars. *Journal of Physical Chemistry C*, **2014**, 118, 22815-22833	3.8	79
356	Identification of descriptors for the CO interaction with metal nanoparticles. *Nano Letters*, **2010**, 10, 1041-5	11.5	79
355	Liquid-Phase Catalytic Transfer Hydrogenation of Furfural over Homogeneous Lewis Acid-Ru/C Catalysts. *ChemSusChem*, **2015**, 8, 2046-54	8.3	77
354	The role of radical wall quenching in flame stability and wall heat flux: hydrogen-air mixtures. *Combustion Theory and Modelling*, **1998**, 2, 515-530	1.5	77
353	From Tree to Tape: Direct Synthesis of Pressure Sensitive Adhesives from Depolymerized Raw Lignocellulosic Biomass. *ACS Central Science*, **2018**, 4, 701-708	16.8	77
352	Overcoming stiffness in stochastic simulation stemming from partial equilibrium: a multiscale Monte Carlo algorithm. *Journal of Chemical Physics*, **2005**, 123, 144114	3.9	76
351	Construction and optimization of complex surface-reaction mechanisms. *AICHE Journal*, **2000**, 46, 2017-2029	3.8	73
350	Kinetic Regime Change in the Tandem Dehydrative Aromatization of Furan Diels–Alder Products. *ACS Catalysis*, **2015**, 5, 2367-2375	13.1	72
349	Correlating Ethylene Glycol Reforming Activity with In Situ EXAFS Detection of Ni Segregation in Supported NiPt Bimetallic Catalysts. *ACS Catalysis*, **2012**, 2, 2290-2296	13.1	72
348	Thermal Management in Catalytic Microreactors. *Industrial & Engineering Chemistry Research*, **2006**, 45, 76-84	3.9	71
347	Coarse-grained stochastic processes and kinetic Monte Carlo simulators for the diffusion of interacting particles. *Journal of Chemical Physics*, **2003**, 119, 9412-9427	3.9	71
346	Diels–Alder cycloaddition of 2-methylfuran and ethylene for renewable toluene. *Applied Catalysis B: Environmental*, **2016**, 180, 487-496	21.8	70
345	Kinetic Modeling of Pt Catalyzed and Computation-Driven Catalyst Discovery for Ethylene Glycol Decomposition. *ACS Catalysis*, **2011**, 1, 1246-1256	13.1	69

344	Silica self-assembly and synthesis of microporous and mesoporous silicates. *Chemistry - A European Journal*, **2006**, 12, 2926-34	4.8	69
343	Ab initio molecular dynamics of hydrogen dissociation on metal surfaces using neural networks and novelty sampling. *Journal of Chemical Physics*, **2007**, 127, 154716	3.9	68
342	Kinetics of faceting of crystals in growth, etching, and equilibrium. *Physical Review B*, **1993**, 47, 4896-4909	3.3	68
341	Biomass-Derived Butadiene by Dehydra-Decyclization of Tetrahydrofuran. *ACS Sustainable Chemistry and Engineering*, **2017**, 5, 3732-3736	8.3	67
340	p-Xylene Formation by Dehydrative Aromatization of a Diels□Alder Product in Lewis and Br□sted Acidic Zeolites. *Journal of Physical Chemistry C*, **2014**, 118, 24415-24424	3.8	67
339	The effect of oxide acidity on HMF etherification. *Catalysis Science and Technology*, **2014**, 4, 3074-3081	5.5	67
338	A DFT study of furan hydrogenation and ring opening on Pd(111). *Green Chemistry*, **2014**, 16, 736-747	10	66
337	A Generalized Approach for Predicting Coverage-Dependent Reaction Parameters of Complex Surface Reactions: Application to H2 Oxidation over Platinum. *Journal of Physical Chemistry A*, **1999**, 103, 8101-8107	2.8	66
336	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	5.3	65
335	Pt catalysts for efficient aerobic oxidation of glucose to glucaric acid in water. *Green Chemistry*, **2016**, 18, 3815-3822	10	64
334	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	3.9	63
333	C□O bond activation using ultralow loading of noble metal catalysts on moderately reducible oxides. *Nature Catalysis*, **2020**, 3, 446-453	36.5	62
332	Conjugation-Driven "Reverse Mars-van Krevelen"-Type Radical Mechanism for Low-Temperature C-O Bond Activation. *Journal of the American Chemical Society*, **2016**, 138, 8104-13	16.4	62
331	Mechanistic Insights into Lewis Acid Metal Salt-Catalyzed Glucose Chemistry in Aqueous Solution. *ACS Catalysis*, **2016**, 6, 1497-1504	13.1	62
330	Tungsten carbides as selective deoxygenation catalysts: experimental and computational studies of converting C3 oxygenates to propene. *Green Chemistry*, **2014**, 16, 761-769	10	62
329	Derivation and validation of mesoscopic theories for diffusion of interacting molecules. *Physical Review Letters*, **2000**, 85, 3898-901	7.4	62
328	Insights into the isomerization of xylose to xylulose and lyxose by a Lewis acid catalyst. *Carbohydrate Research*, **2013**, 368, 89-95	2.9	60
327	CFD Simulations of Coupled, Countercurrent Combustor/Reformer Microdevices for Hydrogen Production. *Industrial & Engineering Chemistry Research*, **2005**, 44, 4982-4992	3.9	60

326	Ignition and extinction of flames near surfaces: Combustion of CH4 in air. *AICHE Journal*, **1994**, 40, 1005-1017	3.6	60
325	Theoretical Approach To Predict the Stability of Supported Single-Atom Catalysts. *ACS Catalysis*, **2019**, 9, 3289-3297	13.1	59
324	Mechanism of Dehydration of Phenols on Noble Metals via First-Principles Microkinetic Modeling. *ACS Catalysis*, **2016**, 6, 3047-3055	13.1	59
323	Mechanistic Study of the Direct Hydrodeoxygenation of m-Cresol over WOx-Decorated Pt/C Catalysts. *ACS Catalysis*, **2018**, 8, 7749-7759	13.1	58
322	Site-Dependent Lewis Acidity of □Al2O3 and Its Impact on Ethanol Dehydration and Etherification. *Journal of Physical Chemistry C*, **2014**, 118, 12899-12907	3.8	58
321	Reactive Deposition of Metal Thin Films within Porous Supports from Supercritical Fluids. *Chemistry of Materials*, **2001**, 13, 2023-2031	9.6	58
320	A perspective on the modeling of biomass processing. *Energy and Environmental Science*, **2012**, 5, 6703	35.4	57
319	Hydrodeoxygenation of HMF over Pt/C in a continuous flow reactor. *AICHE Journal*, **2015**, 61, 590-597	3.6	56
318	Patched bimetallic surfaces are active catalysts for ammonia decomposition. *Nature Communications*, **2015**, 6, 8619	17.4	54
317	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	3.8	53
316	Methane steam reforming at microscales: Operation strategies for variable power output at millisecond contact times. *AICHE Journal*, **2009**, 55, 180-191	3.6	53
315	Plastic waste to fuels by hydrocracking at mild conditions. *Science Advances*, **2021**, 7,	14.3	53
314	Building large microkinetic models with first-principles? accuracy at reduced computational cost. *Chemical Engineering Science*, **2015**, 121, 190-199	4.4	52
313	Insights into the Cr(III) catalyzed isomerization mechanism of glucose to fructose in the presence of water using ab initio molecular dynamics. *Physical Chemistry Chemical Physics*, **2014**, 16, 19564-72	3.6	52
312	Ethanol Activation on Closed-Packed Surfaces. *Industrial & Engineering Chemistry Research*, **2015**, 54, 4213-4225	3.9	52
311	Solventless C□□ Coupling of Low Carbon Furanics to High Carbon Fuel Precursors Using an Improved Graphene Oxide Carbocatalyst. *ACS Catalysis*, **2017**, 7, 3905-3915	13.1	51
310	Br□ste□Evans□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	13.1	51
309	An Efficient Reaction Pathway Search Method Applied to the Decomposition of Glycerol on Platinum. *Journal of Physical Chemistry C*, **2011**, 115, 18707-18720	3.8	51

308	Dominant Reaction Pathways in the Catalytic Partial Oxidation of CH4 on Rh. *Topics in Catalysis*, **2009**, 52, 1983-1988	2.3	50
307	Assessment of Overall Rate Expressions and Multiscale, Microkinetic Model Uniqueness via Experimental Data Injection: Ammonia Decomposition on Ru/Al2O3 for Hydrogen Production. *Industrial & Engineering Chemistry Research*, **2009**, 48, 5255-5265	3.9	50
306	A First Principles-Based Microkinetic Model for the Conversion of Fructose to 5-Hydroxymethylfurfural. *ChemCatChem*, **2012**, 4, 504-511	5.2	49
305	Multiscale modeling reveals poisoning mechanisms of MgO-supported Au clusters in CO oxidation. *Nano Letters*, **2012**, 12, 3621-6	11.5	48
304	DFT-driven multi-site microkinetic modeling of ethanol conversion to ethylene and diethyl ether on Al2O3(1 1 1). *Journal of Catalysis*, **2015**, 323, 121-131	7.3	47
303	Microkinetic Modeling and Reduced Rate Expressions of Ethylene Hydrogenation and Ethane Hydrogenolysis on Platinum. *Industrial & Engineering Chemistry Research*, **2011**, 50, 28-40	3.9	47
302	Time accelerated Monte Carlo simulations of biological networks using the binomial tau-leap method. *Bioinformatics*, **2005**, 21, 2136-7	7.2	47
301	Fundamentals of CO bond activation on metal oxide catalysts. *Nature Catalysis*, **2019**, 2, 269-276	36.5	46
300	Aqueous-phase fructose dehydration using Brønsted acid zeolites: Catalytic activity of dissolved aluminosilicate species. *Applied Catalysis A: General*, **2014**, 469, 116-123	5.1	46
299	Millisecond Methane Steam Reforming Via Process and Catalyst Intensification. *Chemical Engineering and Technology*, **2008**, 31, 1201-1209	2	46
298	Multiscale spatial Monte Carlo simulations: multigriding, computational singular perturbation, and hierarchical stochastic closures. *Journal of Chemical Physics*, **2006**, 124, 64110	3.9	46
297	Carbohydrate dehydration using porous catalysts. *Current Opinion in Chemical Engineering*, **2012**, 1, 312-320	5.1	45
296	Insights into the early stages of metal nanoparticle formation via first-principle calculations: the roles of citrate and water. *Langmuir*, **2008**, 24, 7465-73	4	45
295	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	1.4	45
294	Parameter Optimization of Molecular Models: Application to Surface Kinetics. *Industrial & Engineering Chemistry Research*, **2003**, 42, 1174-1183	3.9	45
293	Computational Insight into the Effect of Sn-Beta Na Exchange and Solvent on Glucose Isomerization and Epimerization. *ACS Catalysis*, **2015**, 5, 5256-5263	13.1	44
292	Catalytic Hydrodeoxygenation of High Carbon Furylmethanes to Renewable Jet-fuel Ranged Alkanes over a Rhenium-Modified Iridium Catalyst. *ChemSusChem*, **2017**, 10, 3225-3234	8.3	44
291	Adipic Acid Production via Metal-Free Selective Hydrogenolysis of Biomass-Derived Tetrahydrofuran-2,5-Dicarboxylic Acid. *ACS Catalysis*, **2017**, 7, 6619-6634	13.1	44

290	Silica nanoparticle formation in the TPAOH-TEOS-H2O system: a population balance model. *Journal of Physical Chemistry B*, **2006**, 110, 3098-108	3.4	44
289	The effects of phase transitions, surface diffusion, and defects on surface catalyzed reactions: Fluctuations and oscillations. *Journal of Chemical Physics*, **1990**, 93, 8306-8313	3.9	44
288	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	3.9	43
287	Spatially adaptive lattice coarse-grained Monte Carlo simulations for diffusion of interacting molecules. *Journal of Chemical Physics*, **2004**, 121, 11420-31	3.9	43
286	Reaction Pathways of Biomass-Derived Oxygenates over Metals and Carbides: From Model Surfaces to Supported Catalysts. *ChemCatChem*, **2015**, 7, 1402-1421	5.2	42
285	Deactivation of Pt/Al2O3 during propane oxidation at low temperatures: Kinetic regimes and platinum oxide formation. *Journal of Catalysis*, **2016**, 337, 122-132	7.3	42
284	Intensification of steam reforming of natural gas: Choosing combustible fuel and reforming catalyst. *Chemical Engineering Science*, **2010**, 65, 398-404	4.4	42
283	Modeling Ignition of Catalytic Reactors with Detailed Surface Kinetics and Transport:Oxidation of H2/Air Mixtures over Platinum Surfaces. *Industrial & Engineering Chemistry Research*, **1997**, 36, 2558-2567	3.9	42
282	Physicochemical Characterization of Silicalite-1 Surface and Its Implications on Crystal Growth. *Langmuir*, **2003**, 19, 4619-4626	4	42
281	Tunable Oleo-Furan Surfactants by Acylation of Renewable Furans. *ACS Central Science*, **2016**, 2, 820-824	16.8	41
280	High vs. low temperature reforming for hydrogen production via microtechnology. *Chemical Engineering Science*, **2009**, 64, 4856-4865	4.4	41
279	Molecular dynamics studies on the role of tetramethylammonium cations in the stability of the silica octamers Si8O20(8-) in solution. *Journal of Physical Chemistry B*, **2005**, 109, 10429-34	3.4	41
278	Multiscale modeling for emergent behavior, complexity, and combinatorial explosion. *AICHE Journal*, **2012**, 58, 1314-1325	3.6	40
277	Extending the region of stable homogeneous micro-combustion through forced unsteady operation. *Proceedings of the Combustion Institute*, **2007**, 31, 3293-3300	5.9	40
276	Two-dimensional detailed modeling of fuel-rich . *Chemical Engineering Science*, **2008**, 63, 2657-2669	4.4	40
275	Structures of small metal clusters. I. Low temperature behavior. *Journal of Chemical Physics*, **1992**, 96, 6880-6890	3.9	40
274	Optimization of the facet structure of transition-metal catalysts applied to the oxygen reduction reaction. *Nature Chemistry*, **2019**, 11, 449-456	17.6	39
273	Spatial modeling of dimerization reaction dynamics in the plasma membrane: Monte Carlo vs. continuum differential equations. *Biophysical Chemistry*, **2006**, 121, 194-208	3.5	39

272	Chemoselective Hydrodeoxygenation of Carboxylic Acids to Hydrocarbons over Nitrogen-Doped Carbon–Alumina Hybrid Supported Iron Catalysts. *ACS Catalysis*, **2019**, 9, 1564-1577	13.1	39
271	Understanding solvent effects on adsorption and protonation in porous catalysts. *Nature Communications*, **2020**, 11, 1060	17.4	38
270	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	13.1	38
269	Theoretical and Experimental Studies of C–C versus C–O Bond Scission of Ethylene Glycol Reaction Pathways via Metal-Modified Molybdenum Carbides. *ACS Catalysis*, **2014**, 4, 1409-1418	13.1	38
268	Fructose-water-dimethylsulfoxide interactions by vibrational spectroscopy and molecular dynamics simulations. *Journal of Physical Chemistry B*, **2012**, 116, 11274-83	3.4	38
267	Equivalence of on-Lattice Stochastic Chemical Kinetics with the Well-Mixed Chemical Master Equation in the Limit of Fast Diffusion. *Computers and Chemical Engineering*, **2011**, 35, 2602-2610	4	38
266	Role of Lewis and Brønsted Acidity in Metal Chloride Catalysis in Organic Media: Reductive Etherification of Furanics. *ACS Catalysis*, **2017**, 7, 7363-7370	13.1	36
265	Catalysis Center for Energy Innovation for Biomass Processing: Research Strategies and Goals. *Catalysis Letters*, **2010**, 140, 77-84	2.8	36
264	Adsorption of the compounds encountered in monosaccharide dehydration in zeolite beta. *Langmuir*, **2013**, 29, 6597-605	4	34
263	Multiscale model for epitaxial growth of films: Growth mode transition. *Physical Review B*, **2001**, 64,	3.3	34
262	Effect of errors in linear scaling relations and Brønsted–Evans–Polanyi relations on activity and selectivity maps. *Journal of Catalysis*, **2016**, 338, 273-283	7.3	34
261	Homogeneous Metal Salt Solutions for Biomass Upgrading and Other Select Organic Reactions. *ACS Catalysis*, **2019**, 9, 9923-9952	13.1	33
260	Solvent-tuned hydrophobicity for faujasite-catalyzed cycloaddition of biomass-derived dimethylfuran for renewable p-xylene. *Green Chemistry*, **2014**, 16, 4086	10	33
259	Durable and self-hydrating tungsten carbide-based composite polymer electrolyte membrane fuel cells. *Nature Communications*, **2017**, 8, 418	17.4	33
258	Dehydration of Glucose to 5-(Hydroxymethyl)furfural and Anhydroglucose: Thermodynamic Insights. *Journal of Physical Chemistry C*, **2012**, 116, 5116-5120	3.8	33
257	Controlling Homogeneous Chemistry in Homogeneous–Heterogeneous Reactors: Application to Propane Combustion. *Industrial & Engineering Chemistry Research*, **2009**, 48, 5962-5968	3.9	33
256	Adsorption in zeolites using mechanically embedded ONIOM clusters. *Physical Chemistry Chemical Physics*, **2016**, 18, 26094-26106	3.6	32
255	Alcohol Adsorption onto Silicalite from Aqueous Solution. *Journal of Physical Chemistry C*, **2011**, 115, 18659-18669	3.8	32

254	What controls au nanoparticle dispersity during growth?. *Nano Letters*, **2010**, 10, 3408-13	11.5	31
253	From microscopic interactions to macroscopic laws of cluster evolution. *Physical Review Letters*, **2000**, 84, 1511-4	7.4	31
252	Renewable lubricants with tailored molecular architecture. *Science Advances*, **2019**, 5, eaav5487	14.3	30
251	Infrared spectroscopy data- and physics-driven machine learning for characterizing surface microstructure of complex materials. *Nature Communications*, **2020**, 11, 1513	17.4	30
250	Kinetic regimes in the tandem reactions of H-BEA catalyzed formation of p-xylene from dimethylfuran. *Catalysis Science and Technology*, **2016**, 6, 178-187	5.5	30
249	On the Brønsted acid-catalyzed homogeneous hydrolysis of furans. *ChemSusChem*, **2013**, 6, 2066-8	8.3	30
248	Heterogeneities in EGF receptor density at the cell surface can lead to concave up scatchard plot of EGF binding. *FEBS Letters*, **2005**, 579, 3043-7	3.8	30
247	DFT Study of the Conversion of Furfuryl Alcohol to 2-Methylfuran on RuO2 (110). *Journal of Physical Chemistry C*, **2015**, 119, 5938-5945	3.8	29
246	Novel micromixers driven by flow instabilities: Application to post-reactors. *AICHE Journal*, **2005**, 51, 3193-3204	3.6	29
245	Ultrafast flow chemistry for the acid-catalyzed conversion of fructose. *Energy and Environmental Science*, **2019**, 12, 2463-2475	35.4	28
244	Molecular screening of alcohol and polyol adsorption onto MFI-type zeolites. *Langmuir*, **2012**, 28, 4491-94		28
243	Scale-out of Microreactor Stacks for Portable and Distributed Processing: Coupling of Exothermic and Endothermic Processes for Syngas Production. *Industrial & Engineering Chemistry Research*, **2010**, 49, 10942-10955	3.9	28
242	Spectral Methods for Mesoscopic Models of Pattern Formation. *Journal of Computational Physics*, **2001**, 173, 364-390	4.1	28
241	Validation of mesoscopic theory and its application to computing concentration dependent diffusivities. *Journal of Chemical Physics*, **2001**, 115, 11278-11288	3.9	28
240	Acylation of methylfuran with Brønsted and Lewis acid zeolites. *Applied Catalysis A: General*, **2018**, 564, 90-101	5.1	27
239	Reactive adsorption for the selective dehydration of sugars to furans: Modeling and experiments. *AICHE Journal*, **2013**, 59, 3378-3390	3.6	27
238	Millisecond Production of Hydrogen from Alternative, High Hydrogen Density Fuels in a Cocurrent Multifunctional Microreactor. *Industrial & Engineering Chemistry Research*, **2009**, 48, 1749-1760	3.9	27
237	Stochastic simulations of ErbB homo and heterodimerisation: potential impacts of receptor conformational state and spatial segregation. *IET Systems Biology*, **2008**, 2, 256-72	1.4	27

236	Self-assembly and phase behavior of germanium oxide nanoparticles in basic aqueous solutions. *Langmuir*, **2007**, 23, 2784-91	4	27
235	Design Principles of Heteroepitaxial Bimetallic Catalysts. *ACS Catalysis*, **2013**, 3, 2248-2255	13.1	26
234	Experimental and theoretical studies of ammonia decomposition activity on Fe-Pt, Co-Pt, and Cu-Pt bimetallic surfaces. *Journal of Chemical Physics*, **2011**, 134, 184701	3.9	26
233	Bifurcation analysis of Liesegang ring pattern formation. *Physical Review Letters*, **2004**, 92, 088301	7.4	26
232	Reaction Pathways and Intermediates in Selective Ring Opening of Biomass-Derived Heterocyclic Compounds by Iridium. *ACS Catalysis*, **2016**, 6, 7002-7009	13.1	26
231	Distribution of open sites in Sn-Beta zeolite. *Microporous and Mesoporous Materials*, **2017**, 245, 45-50	5.3	25
230	Nanoporous CuAlCo Alloys for Selective Furfural Hydrodeoxygenation to 2-Methylfuran. *Industrial & Engineering Chemistry Research*, **2017**, 56, 3866-3872	3.9	25
229	Ring Activation of Furanic Compounds on Ruthenium-Based Catalysts. *Journal of Physical Chemistry C*, **2015**, 119, 6075-6085	3.8	25
228	Group Additivity for Aqueous Phase Thermochemical Properties of Alcohols on Pt(111). *Journal of Physical Chemistry C*, **2017**, 121, 21510-21519	3.8	25
227	A Combined DFT and Statistical Mechanics Study for the CO Oxidation on the Au10 Cluster. *Journal of Physical Chemistry C*, **2011**, 115, 20192-20200	3.8	25
226	Initial stages of self-organization of silica-alumina gels in zeolite synthesis. *Langmuir*, **2007**, 23, 4532-40	4	25
225	Understanding the differences between microporous and mesoporous synthesis through the phase behavior of silica. *Microporous and Mesoporous Materials*, **2006**, 90, 102-111	5.3	25
224	Computational modeling reveals molecular details of epidermal growth factor binding. *BMC Cell Biology*, **2005**, 6, 41		25
223	Ring-Opening Reaction of Furfural and Tetrahydrofurfuryl Alcohol on Hydrogen-Predosed Iridium(1 1 1) and Cobalt/Iridium(1 1 1) Surfaces. *ChemCatChem*, **2017**, 9, 1701-1707	5.2	24
222	First-Principles Kinetic and Spectroscopic Insights into Single-Atom Catalysis. *ACS Catalysis*, **2019**, 9, 5002-5010	13.1	24
221	Group Additivity and Modified Linear Scaling Relations for Estimating Surface Thermochemistry on Transition Metal Surfaces: Application to Furanics. *Journal of Physical Chemistry C*, **2015**, 119, 10417-10426	3.8	24
220	Adsorption of HMF from water/DMSO solutions onto hydrophobic zeolites: experiment and simulation. *ChemSusChem*, **2014**, 7, 236-44	8.3	24
219	Roles of thermal and radical quenching in emissions of wall-stabilized hydrogen flames. *AICHE Journal*, **1998**, 44, 2025-2034	3.6	24

218	Microscopic simulation of membrane molecule diffusion on corralled membrane surfaces. *Biophysical Journal*, **2008**, 94, 1551-64	2.9	24
217	Thermodynamics of Silica Nanoparticle Self-Assembly in Basic Solutions of Monovalent Cations. *Journal of Physical Chemistry C*, **2008**, 112, 14754-14761	3.8	24
216	Catalysis at the sub-nanoscale: complex CO oxidation chemistry on a few Au atoms. *Catalysis Science and Technology*, **2015**, 5, 134-141	5.5	23
215	Molybdenum Oxide-Modified Iridium Catalysts for Selective Production of Renewable Oils for Jet and Diesel Fuels and Lubricants. *ACS Catalysis*, **2019**, 9, 7679-7689	13.1	23
214	Group Additivity for Estimating Thermochemical Properties of Furanic Compounds on Pd(111). *Industrial & Engineering Chemistry Research*, **2014**, 53, 11929-11938	3.9	23
213	Growth mechanisms of metal nanoparticles via first principles. *Physical Review Letters*, **2009**, 102, 155505	7.4	23
212	Bifurcation Behavior of Premixed Hydrogen/Air Mixtures in a Continuous Stirred Tank Reactor. *Combustion Science and Technology*, **1995**, 109, 347-371	1.5	23
211	Coupled stochastic spatial and non-spatial simulations of ErbB1 signaling pathways demonstrate the importance of spatial organization in signal transduction. *PLoS ONE*, **2009**, 4, e6316	3.7	23
210	Effect of Substitutionally Doped Graphene on the Activity of Metal Nanoparticle Catalysts for the Hydrogen Oxidation Reaction. *ACS Catalysis*, **2019**, 9, 1129-1139	13.1	23
209	Tandem Diels–Alder Reaction of Dimethylfuran and Ethylene and Dehydration to para-Xylene Catalyzed by Zeotypic Lewis Acids. *ChemCatChem*, **2017**, 9, 2523-2535	5.2	22
208	Acceleration and sensitivity analysis of lattice kinetic Monte Carlo simulations using parallel processing and rate constant rescaling. *Journal of Chemical Physics*, **2017**, 147, 164103	3.9	22
207	Thermochemistry of gas-phase and surface species via LASSO-assisted subgraph selection. *Reaction Chemistry and Engineering*, **2018**, 3, 454-466	4.9	22
206	Adipic acid production catalyzed by a combination of a solid acid and an iodide salt from biomass-derived tetrahydrofuran-2,5-dicarboxylic acid. *Catalysis Science and Technology*, **2018**, 8, 2661-2671	5.5	22
205	Error estimates in semi-empirical estimation methods of surface reactions. *Journal of Catalysis*, **2013**, 297, 202-216	7.3	22
204	Experiments and computations of microfluidic liquid–liquid flow patterns. *Reaction Chemistry and Engineering*, **2020**, 5, 39-50	4.9	22
203	Polypropylene Plastic Waste Conversion to Lubricants over Ru/TiO2 Catalysts. *ACS Catalysis*, **2021**, 11, 8104-8115	13.1	22
202	Insights into the Ring-Opening of Biomass-Derived Furanics over Carbon-Supported Ruthenium. *ChemSusChem*, **2016**, 9, 3113-3121	8.3	22
201	Recent advances in understanding the pH dependence of the hydrogen oxidation and evolution reactions. *Journal of Catalysis*, **2018**, 367, 328-331	7.3	22

200	Understanding Acidity of Molten Salt Hydrate Media for Cellulose Hydrolysis by Combining Kinetic Studies, Electrolyte Solution Modeling, Molecular Dynamics Simulations, and 13C NMR Experiments. *ACS Catalysis*, **2019**, 9, 10551-10561	13.1	21
199	Tuning cellulose pyrolysis chemistry: selective decarbonylation via catalyst-impregnated pyrolysis. *Catalysis Science and Technology*, **2014**, 4, 3822-3825	5.5	21
198	Comparison of ignition strategies for catalytic microburners. *Proceedings of the Combustion Institute*, **2009**, 32, 3027-3034	5.9	21
197	Coarse-grained kinetic Monte Carlo models: Complex lattices, multicomponent systems, and homogenization at the stochastic level. *Journal of Chemical Physics*, **2008**, 129, 184101	3.9	21
196	Partial oxidation of light alkanes in short contact time microreactors. *Catalysis*,98-137	1.6	21
195	A Python Multiscale Thermochemistry Toolbox (pMuTT) for thermochemical and kinetic parameter estimation. *Computer Physics Communications*, **2020**, 247, 106864	4.2	21
194	The Future is Garbage: Repurposing of Food Waste to an Integrated Biorefinery. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 8124-8136	8.3	20
193	The origin of selectivity in the conversion of glucose to fructose and mannose in Sn-BEA and Na-exchanged Sn-BEA zeolites. *Journal of Catalysis*, **2017**, 355, 11-16	7.3	20
192	Liquid-phase dehydration of propylene glycol using solid-acid catalysts. *Applied Catalysis A: General*, **2012**, 449, 59-68	5.1	20
191	Efficient gradient estimation using finite differencing and likelihood ratios for kinetic Monte Carlo simulations. *Journal of Computational Physics*, **2012**, 231, 7170-7186	4.1	20
190	Effect of oxide support surface area on hydrogenation activity: Pt/Ni bimetallic catalysts supported on low and high surface area Al2O3 and ZrO2. *Applied Catalysis A: General*, **2011**, 408, 87-95	5.1	20
189	Recent Advances in the Photocatalytic Conversion of Biomass-Derived Furanic Compounds. *ACS Catalysis*, **2021**, 11, 11336-11359	13.1	20
188	General Acid-Type Catalysis in the Dehydrative Aromatization of Furans to Aromatics in H-[Al]-BEA, H-[Fe]-BEA, H-[Ga]-BEA, and H-[B]-BEA Zeolites. *Journal of Physical Chemistry C*, **2017**, 121, 13666-13679	3.8	19
187	Inhibition of Xylene Isomerization in the Production of Renewable Aromatic Chemicals from Biomass-Derived Furans. *ACS Catalysis*, **2016**, 6, 2076-2088	13.1	19
186	Production of high-yield short-chain oligomers from cellulose via selective hydrolysis in molten salt hydrates and separation. *Green Chemistry*, **2019**, 21, 5030-5038	10	19
185	Microkinetic modeling of Pt-catalyzed ethylene glycol steam reforming. *Applied Catalysis A: General* , **2012**, 431-432, 18-24	5.1	19
184	Correlating the Surface Chemistry of C2 and C3 Aldoses with a C6 Sugar: Reaction of Glucose, Glyceraldehyde, and Glycolaldehyde on Pd(111). *Journal of Physical Chemistry C*, **2012**, 116, 18891-18898	3.8	19
183	Microkinetic modeling of the fast selective catalytic reduction of nitrogen oxide with ammonia on H-ZSM5 based on first principles. *Journal of Catalysis*, **2011**, 283, 178-191	7.3	19

182	Enhancing stability in parallel plate microreactor stacks for syngas production. *Chemical Engineering Science*, **2011**, 66, 1051-1059	4.4	19
181	Structures of small metal clusters. II. Phase transitions and isomerization. *Journal of Chemical Physics*, **1992**, 96, 6891-6901	3.9	19
180	From Density Functional Theory to Microchemical Device Homogenization: Model Prediction of Hydrogen Production For Portable Fuel Cells. *International Journal for Multiscale Computational Engineering*, **2004**, 2, 221-238	2.4	19
179	Effect of oxide supports in stabilizing desirable Pt-Ni bimetallic structures for hydrogenation and reforming reactions. *Physical Chemistry Chemical Physics*, **2013**, 15, 12156-64	3.6	18
178	Effect of local metal microstructure on adsorption on bimetallic surfaces: atomic nitrogen on Ni/Pt(111). *Journal of Chemical Physics*, **2013**, 138, 174702	3.9	18
177	The Effects of the MgO Support and Alkali Doping on the CO Interaction with Au. *Journal of Physical Chemistry C*, **2009**, 113, 7329-7335	3.8	18
176	Understanding mixing of Ni and Pt in the Ni/Pt(111) bimetallic catalyst via molecular simulation and experiments. *Journal of Chemical Physics*, **2010**, 133, 224503	3.9	18
175	Hierarchical Reduced Models for Catalytic Combustion: H2/Air Mixtures Near Platinum Surfaces. *Combustion Science and Technology*, **1997**, 129, 243-275	1.5	18
174	A hybrid multiscale Monte Carlo algorithm (HyMSMC) to cope with disparity in time scales and species populations in intracellular networks. *BMC Bioinformatics*, **2007**, 8, 175	3.6	18
173	The Catalytic Mechanics of Dynamic Surfaces: Stimulating Methods for Promoting Catalytic Resonance. *ACS Catalysis*, **2020**, 10, 12666-12695	13.1	18
172	Catalytic production of renewable lubricant base oils from bio-based 2-alkylfurans and enals. *Green Chemistry*, **2019**, 21, 3606-3614	10	17
171	Potential of mean force for tetramethylammonium binding to cagelike oligosilicates in aqueous solution. *Journal of the American Chemical Society*, **2006**, 128, 16138-47	16.4	17
170	Reductive catalytic fractionation of agricultural residue and energy crop lignin and application of lignin oil in antimicrobials. *Green Chemistry*, **2020**, 22, 7435-7447	10	17
169	Stability of heterogeneous single-atom catalysts: a scaling law mapping thermodynamics to kinetics. *Npj Computational Materials*, **2020**, 6,	10.9	17
168	Direct speciation methods to quantify catalytically active species of AlCl in glucose isomerization.. *RSC Advances*, **2018**, 8, 17101-17109	3.7	17
167	Dehydra-Decyclization of Tetrahydrofuran on H-ZSM5: Mechanisms, Pathways, and Transition State Entropy. *ACS Catalysis*, **2019**, 9, 10279-10293	13.1	16
166	Lattice Convolutional Neural Network Modeling of Adsorbate Coverage Effects. *Journal of Physical Chemistry C*, **2019**, 123, 18951-18959	3.8	16
165	Scaling relationships and theory for vibrational frequencies of adsorbates on transition metal surfaces. *Nature Communications*, **2017**, 8, 1842	17.4	16

164	Parametric sensitivity analysis for biochemical reaction networks based on pathwise information theory. *BMC Bioinformatics*, **2013**, 14, 311	3.6	16
163	Ammonia decomposition activity on monolayer Ni supported on Ru, Pt and WC substrates. *Surface Science*, **2011**, 605, 2055-2060	1.8	16
162	Modeling Silica Nanoparticle Dissolution in TPAOH□TEOS□H2O Solutions. *Journal of Physical Chemistry C*, **2008**, 112, 14769-14775	3.8	16
161	Temporal acceleration of spatially distributed kinetic Monte Carlo simulations. *Journal of Computational Physics*, **2006**, 211, 596-615	4.1	16
160	A Review of Biorefinery Separations for Bioproduct Production via Thermocatalytic Processing. *Annual Review of Chemical and Biomolecular Engineering*, **2017**, 8, 115-137	8.9	15
159	Comparison of Ethylene Glycol Steam Reforming Over Pt and NiPt Catalysts on Various Supports. *Topics in Catalysis*, **2013**, 56, 1644-1650	2.3	15
158	High-Temperature Decomposition of Br□sted Acid Sites in Gallium-Substituted Zeolites. *Journal of Physical Chemistry C*, **2010**, 114, 19395-19405	3.8	15
157	Kinetically driven instabilities and selectivities in methane oxidation. *AICHE Journal*, **1997**, 43, 2083-2095	3.6	15
156	Molecular dynamics study of the stabilization of the silica hexamer Si6O15(6-) in aqueous and methanolic solutions. *Journal of Physical Chemistry B*, **2008**, 112, 7-10	3.4	15
155	Modeling of zeolite L crystallization using continuum time Monte Carlo simulations. *Journal of Chemical Physics*, **1999**, 111, 2143-2150	3.9	15
154	Polyethylene Hydrogenolysis at Mild Conditions over Ruthenium on Tungstated Zirconia. *Jacs Au*, **2021**, 1, 1422-1434		15
153	Group Additivity for Thermochemical Property Estimation of Lignin Monomers on Pt(111). *Journal of Physical Chemistry C*, **2016**, 120, 19234-19241	3.8	14
152	Operation regimes in catalytic combustion: H2/air mixtures near Pt. *AICHE Journal*, **1998**, 44, 2035-2043	3.6	14
151	Systems tasks in nanotechnology via hierarchical multiscale modeling: Nanopattern formation in heteroepitaxy. *Chemical Engineering Science*, **2007**, 62, 4852-4863	4.4	14
150	A Complete Pressure□Temperature Diagram for Air Oxidation of Hydrogen in a Continuous-Flow Stirred Tank Reactor. *Journal of Physical Chemistry A*, **1999**, 103, 7990-7999	2.8	14
149	Scaleup of a Single-Mode Microwave Reactor. *Industrial & Engineering Chemistry Research*, **2020**, 59, 2516-2523	3.9	14
148	Branched Bio-Lubricant Base Oil Production through Aldol Condensation. *ChemSusChem*, **2019**, 12, 4780-4785	3	13
147	Microkinetic Modeling of Ethane Total Oxidation on Pt. *Industrial & Engineering Chemistry Research*, **2014**, 53, 10051-10058	3.9	13

146	Temporal coarse-graining of microscopic-lattice kinetic Monte Carlo simulations via tau leaping. *Physical Review E*, **2008**, 78, 046713	2.4	13
145	Multiscale hybrid modeling of film deposition within porous substrates. *AICHE Journal*, **2004**, 50, 684-695	3.6	13
144	Steady state likelihood ratio sensitivity analysis for stiff kinetic Monte Carlo simulations. *Journal of Chemical Physics*, **2015**, 142, 044108	3.9	12
143	Catalytic resonance theory: parallel reaction pathway control. *Chemical Science*, **2020**, 11, 3501-3510	9.4	12
142	On the oligomerization mechanism of Br□sted acid-catalyzed conversion of furans to diesel-range fuels. *Applied Catalysis A: General*, **2014**, 485, 118-122	5.1	12
141	Selective hydrodeoxygenation of tartaric acid to succinic acid. *Catalysis Science and Technology*, **2017**, 7, 4944-4954	5.5	12
140	Density Functional Theory Study of Methane Oxidation and Reforming on Pt(111) and Pt(211). *Industrial & Engineering Chemistry Research*, **2012**, 120918084645004	3.9	12
139	Predicting the adsorption behavior in bulk from metal clusters. *Chemical Physics Letters*, **2011**, 518, 99-103	2.5	12
138	A Fast Approach to Predictive Models: NO-Oxidation in Exhaust Gas Aftertreatment Systems. *Topics in Catalysis*, **2009**, 52, 1925-1928	2.3	12
137	Spatially adaptive grand canonical ensemble Monte Carlo simulations. *Physical Review E*, **2005**, 71, 026702	2.4	12
136	The role of macroscopic transport phenomena in film microstructure during epitaxial growth. *Applied Physics Letters*, **1999**, 74, 2797-2799	3.4	12
135	Products in methane combustion near surfaces. *AICHE Journal*, **1994**, 40, 1018-1025	3.6	12
134	Explainable and trustworthy artificial intelligence for correctable modeling in chemical sciences. *Science Advances*, **2020**, 6,	14.3	12
133	Methyl-ligated tin silsesquioxane catalyzed reactions of glucose. *Journal of Catalysis*, **2016**, 341, 62-71	7.3	12
132	Microkinetic Modeling and Reduced Rate Expression of the Water□as Shift Reaction on Nickel. *Industrial & Engineering Chemistry Research*, **2018**, 57, 10269-10280	3.9	12
131	Parallelization of tau-leap coarse-grained Monte Carlo simulations on GPUs **2010**,		11
130	Hybrid quantum mechanics/molecular mechanics-based molecular dynamics simulation of acid-catalyzed dehydration of polyols in liquid water. *Journal of Physical Chemistry A*, **2011**, 115, 8816-21	2.8	11
129	Molecular dynamics of hydrogen dissociation on an oxygen covered Pt(111) surface. *Journal of Chemical Physics*, **2008**, 128, 154708	3.9	11

128	The roles of supersaturation, terrace width, and impurities on the formation of macrosteps on crystal surfaces using the terrace-ledge-kink model. *Surface Science*, **1992**, 262, 359-370	1.8	11
127	Solvent selection for biphasic extraction of 5-hydroxymethylfurfural via multiscale modeling and experiments. *Green Chemistry*, **2020**, 22, 8699-8712	10	11
126	Process Systems Engineering Perspective on the Design of Materials and Molecules. *Industrial & Engineering Chemistry Research*, **2021**, 60, 5194-5206	3.9	11
125	Liquid□liquid Microfluidic Flows for Ultrafast 5-Hydroxymethyl Furfural Extraction. *Industrial & Engineering Chemistry Research*, **2021**, 60, 3723-3735	3.9	11
124	Biomass-derived oxygenate reforming on Pt(111): A demonstration of surface science using d-glucose and its model surrogate glycolaldehyde. *Surface Science*, **2012**, 606, L91-L94	1.8	10
123	Homogenization of mesoscopic theories: Effective properties of model membranes. *AICHE Journal*, **2002**, 48, 1083-1092	3.6	10
122	Periodic patterning in materials deposition by self-regulating diffusion-reaction processes. *Applied Physics Letters*, **2003**, 82, 3357-3359	3.4	10
121	Theoretical Study of Ethylene Hydroformylation on Atomically Dispersed Rh/Al2O3 Catalysts: Reaction Mechanism and Influence of the ReOx Promoter. *ACS Catalysis*, **2021**, 11, 9506-9518	13.1	10
120	Ethane Dehydrogenation on Single and Dual Centers of Ga-modified □Al2O3. *ACS Catalysis*, **2021**, 11, 1380-1391	13.1	10
119	A review of thermal and thermocatalytic valorization of food waste. *Green Chemistry*, **2021**, 23, 2806-2833	10	10
118	Kinetic Studies of Acid Hydrolysis of Food Waste-Derived Saccharides. *Industrial & Engineering Chemistry Research*, **2018**, 57, 17365-17374	3.9	10
117	Catalytic Hydrotreatment of Humins to Bio-Oil in Methanol over Supported Metal Catalysts. *ChemSusChem*, **2018**, 11, 3609-3617	8.3	10
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	21.8	10
115	Phosphonate-Modified UiO-66 Br□sted Acid Catalyst and Its Use in Dehydra-Decyclization of 2-Methyltetrahydrofuran to Pentadienes. *Angewandte Chemie - International Edition*, **2020**, 59, 13260-13266	16.4	9
114	Growth kinetics of humins studied via X-ray scattering. *Green Chemistry*, **2020**, 22, 2301-2309	10	9
113	Cooperative Catalysis by Surface Lewis Acid/Silanol for Selective Fructose Etherification on Sn-SPP Zeolite. *ACS Catalysis*, **2018**, 8, 9056-9065	13.1	9
112	Multilevel coarse graining and nano-pattern discovery in many particle stochastic systems. *Journal of Computational Physics*, **2012**, 231, 2599-2620	4.1	9
111	Kinetic modeling of Pt-catalyzed glycolaldehyde decomposition to syngas. *Journal of Physical Chemistry A*, **2012**, 116, 4621-8	2.8	9

110	Long-time integration methods for mesoscopic models of pattern-forming systems. *Journal of Computational Physics*, **2011**, 230, 5704-5715	4.1	9
109	Pattern Formation in Porous Media via the Liesegang Ring Mechanism. *Industrial & Engineering Chemistry Research*, **2004**, 43, 3073-3084	3.9	9
108	Multiscale Modeling Combined with Active Learning for Microstructure Optimization of Bifunctional Catalysts. *Industrial & Engineering Chemistry Research*, **2019**, 58, 6146-6154	3.9	9
107	Microkinetic modeling of aqueous phase biomass conversion: Application to ethylene glycol reforming. *Chemical Engineering Science*, **2019**, 197, 415-418	4.4	9
106	Fast microflow kinetics and acid catalyst deactivation in glucose conversion to 5-hydroxymethylfurfural. *Reaction Chemistry and Engineering*, **2021**, 6, 152-164	4.9	9
105	Spectroscopic characterization of a highly selective NiCu3/C hydrodeoxygenation catalyst. *Catalysis Science and Technology*, **2018**, 8, 6100-6108	5.5	9
104	Tandem Aromatization of Oxygenated Furans by Framework Zinc In Zeolites. A Computational Study. *Journal of Physical Chemistry C*, **2017**, 121, 22178-22186	3.8	8
103	Operation and Optimization of Microwave-Heated Continuous-Flow Microfluidics. *Industrial & Engineering Chemistry Research*, **2020**, 59, 10418-10427	3.9	8
102	Adaptive coarse-grained Monte Carlo simulation of reaction and diffusion dynamics in heterogeneous plasma membranes. *BMC Bioinformatics*, **2010**, 11, 218	3.6	8
101	The role of molecular interactions and interfaces in diffusion: transport diffusivity and evaluation of the Darken approximation. *Journal of Chemical Physics*, **2005**, 123, 184707	3.9	8
100	Downsizing Chemical Processes for Portable Hydrogen Production. *ACS Symposium Series*, **2005**, 179-193	0.4	8
99	Spontaneous Formation of Periodically Patterned Deposits by Chemical Vapor Deposition. *Journal of the American Chemical Society*, **2000**, 122, 12864-12865	16.4	8
98	Comparison of small metal clusters: Ni, Pd, Pt, Cu, Ag, Au. *Zeitschrift F□ Physik D-Atoms Molecules and Clusters*, **1993**, 26, 156-158		8
97	Hydrodeoxygenation of m-Cresol Over Pt-WOx/C Using H2 Generated In Situ by n-Hexane Dehydrogenation. *Catalysis Letters*, **2020**, 150, 913-921	2.8	8
96	Surface chemistry dictates stability and oxidation state of supported single metal catalyst atoms. *Chemical Science*, **2020**, 11, 1469-1477	9.4	8
95	Finite-Temperature Structures of Supported Subnanometer Catalysts Inferred Statistical Learning and Genetic Algorithm-Based Optimization. *ACS Nano*, **2020**, 14, 13995-14007	16.7	8
94	Active learning-driven quantitative synthesis□structure□roperty relations for improving performance and revealing active sites of nitrogen-doped carbon for the hydrogen evolution reaction. *Reaction Chemistry and Engineering*, **2020**, 5, 2134-2147	4.9	8
93	Stochastic averaging and sensitivity analysis for two scale reaction networks. *Journal of Chemical Physics*, **2016**, 144, 074104	3.9	8

92	One-step lignocellulose depolymerization and saccharification to high sugar yield and less condensed isolated lignin. *Green Chemistry*, **2021**, 23, 1200-1211	10	8
91	Multiscale modeling of microwave-heated multiphase systems. *Chemical Engineering Journal*, **2020**, 397, 125262	14.7	7
90	Characterization of Oxidation States in Metal/Metal Oxide Catalysts in Liquid-Phase Hydrodeoxygenation Reactions with a Trickle Bed Reactor. *Industrial & Engineering Chemistry Research*, **2018**, 57, 5591-5598	3.9	7
89	Poisoning of Ru/C by homogeneous Brønsted acids in hydrodeoxygenation of 2,5-dimethylfuran via catalytic transfer hydrogenation. *Applied Catalysis A: General*, **2017**, 542, 327-335	5.1	7
88	1,2-H- versus 1,2-C-Shift on Sn-Silsesquioxanes. *ACS Catalysis*, **2017**, 7, 25-33	13.1	7
87	Design and Fabrication of a High-Throughput Microreactor and Its Evaluation for Highly Exothermic Reactions. *Industrial & Engineering Chemistry Research*, **2012**, 51, 16270-16277	3.9	7
86	Computational-based catalyst design for thermochemical transformations. *MRS Bulletin*, **2011**, 36, 211-215	3.5	7
85	Adsorption and Diffusion of Methanol, Glycerol, and Their Mixtures in a Metal Organic Framework. *Industrial & Engineering Chemistry Research*, **2011**, 50, 14084-14089	3.9	7
84	Nanoscale surface pattern evolution in heteroepitaxial bimetallic films. *ACS Nano*, **2011**, 5, 7168-75	16.7	7
83	Catalytic Partial Oxidation Pilot Plant Study. *Industrial & Engineering Chemistry Research*, **2010**, 49, 94-103	3.9	7
82	Catalytic Adipic Acid Production on Zeolites from Biomass-Derived Tetrahydrofuran-2,5-dicarboxylic Acid. *ACS Applied Energy Materials*, **2020**, 3, 99-105	6.1	7
81	Ethylene production by direct conversion of methane over isolated single active centers. *Chemical Engineering Journal*, **2021**, 420, 130493	14.7	7
80	Temperature Homogeneity under Selective and Localized Microwave Heating in Structured Flow Reactors. *Industrial & Engineering Chemistry Research*, **2021**, 60, 6835-6847	3.9	7
79	Oxidation of aromatic oxygenates for the production of terephthalic acid. *Applied Catalysis A: General*, **2018**, 552, 98-104	5.1	6
78	Non-parametric correlative uncertainty quantification and sensitivity analysis: Application to a Langmuir bimolecular adsorption model. *AIP Advances*, **2018**, 8, 035021	1.5	6
77	Volcano Curves for in Silico Prediction of Mono- and Bifunctional Catalysts: Application to Ammonia Decomposition. *Journal of Physical Chemistry C*, **2019**, 123, 27097-27104	3.8	6
76	On factors controlling activity of submonolayer bimetallic catalysts: nitrogen desorption. *Journal of Chemical Physics*, **2014**, 140, 014703	3.9	6
75	Core–Shell Nanocatalyst Design by Combining High-Throughput Experiments and First-Principles Simulations. *ChemCatChem*, **2013**, 5, 3712-3718	5.2	6

74	Solvent-induced frequency shifts of 5-hydroxymethylfurfural deduced via infrared spectroscopy and ab initio calculations. *Journal of Physical Chemistry A*, **2014**, 118, 12149-60	2.8	6
73	Synthesis of mesoporous silica nanobamboo with highly dispersed tungsten carbide nanoparticles. *Dalton Transactions*, **2012**, 41, 6914-8	4.3	6
72	Nonlinear dynamics of surface stabilized premixed and diffusion flames: current trends and future directions. *Chemical Engineering Science*, **2000**, 55, 311-319	4.4	6
71	Numerical Assessment of Theoretical Error Estimates in Coarse-Grained Kinetic Monte Carlo Simulations: Application to Surface Diffusion. *International Journal for Multiscale Computational Engineering*, **2005**, 3, 59-70	2.4	6
70	An unconventional DCOx favored Co/N-C catalyst for efficient conversion of fatty acids and esters to liquid alkanes. *Applied Catalysis A: General*, **2020**, 591, 117385	5.1	6
69	Thiol-promoted catalytic synthesis of high-performance furan-containing lubricant base oils from biomass derived 2-alkylfurans and ketones. *Green Chemistry*, **2020**, 22, 7896-7906	10	6
68	Synthesis of rigid and stable large-inner-diameter multiwalled carbon nanotubes. *RSC Advances*, **2012**, 2, 2685	3.7	5
67	Roles of Transients and Nucleation in Film Deposition within a Support. *Industrial & Engineering Chemistry Research*, **2003**, 42, 1321-1328	3.9	5
66	Complex dynamics of combustion flows by direct numerical simulations. *Physics of Fluids*, **2000**, 12, 252-255	4.4	5
65	A Review of Microwave-assisted Process Intensified Multiphase Reactors. *Chemical Engineering Journal*, **2021**, 133183	14.7	5
64	Extraction of Furfural and Furfural/5-Hydroxymethylfurfural from Mixed Lignocellulosic Biomass-Derived Feedstocks. *ACS Sustainable Chemistry and Engineering*, **2021**, 9, 7489-7498	8.3	5
63	Intensified microwave-assisted heterogeneous catalytic reactors for sustainable chemical manufacturing. *Chemical Engineering Journal*, **2021**, 420, 130476	14.7	5
62	Intensified reactive extraction for the acid-catalyzed conversion of fructose to 5-hydroxymethyl furfural. *Chemical Engineering Journal*, **2022**, 428, 132556	14.7	5
61	Modulating the dynamics of Brønsted acid sites on PtWOx inverse catalyst. *Nature Catalysis*, **2022**, 5, 144-153	36.5	5
60	Reaction Network Viewer (ReNView): An open-source framework for reaction path visualization of chemical reaction systems. *SoftwareX*, **2020**, 11, 100442	2.7	4
59	Continuum mesoscopic framework for multiple interacting species and processes on multiple site types and/or crystallographic planes. *Journal of Chemical Physics*, **2007**, 127, 034705	3.9	4
58	Molecular sieve valves driven by adsorbate-adsorbate interactions: hysteresis in permeation of microporous membranes. *Journal of Chemical Physics*, **2005**, 122, 204706	3.9	4
57	Instabilities in homogeneous nonisothermal reactors: Comparison of deterministic and Monte Carlo simulations. *Journal of Chemical Physics*, **1995**, 102, 1781-1790	3.9	4

56	Ambient-pressure lignin valorization to high-performance polymers by intensified reductive catalytic deconstruction.. *Science Advances*, **2022**, 8, eabj7523	14.3	4
55	Polyolefin plastic waste hydroconversion to fuels, lubricants, and waxes: a comparative study. *Reaction Chemistry and Engineering*,	4.9	4
54	Experimental Insights into the Coupling of Methane Combustion and Steam Reforming in a Catalytic Plate Reactor in Transient Mode. *Industrial & Engineering Chemistry Research*, **2021**, 60, 196-209	3.9	4
53	Spectroscopic Probe Molecule Selection Using Quantum Theory, First-Principles Calculations, and Machine Learning. *ACS Nano*, **2020**,	16.7	4
52	Mechanism of Br□sted Acid-Catalyzed Glucose Dehydration. *ChemSusChem*, **2015**, 8, 1291-1291	8.3	3
51	Mesoscopic Modeling of Surface Processes. *The IMA Volumes in Mathematics and Its Applications*, **2004**, 179-198	0.5	3
50	The role of molecular interactions and interfaces in diffusion: permeation through single-crystal and polycrystalline microporous membranes. *Journal of Chemical Physics*, **2005**, 123, 184708	3.9	3
49	Catalytic resonance of ammonia synthesis by simulated dynamic ruthenium crystal strain.. *Science Advances*, **2022**, 8, eabl6576	14.3	3
48	NEXTorch: A Design and Bayesian Optimization Toolkit for Chemical Sciences and Engineering. *Journal of Chemical Information and Modeling*, **2021**, 61, 5312-5319	6.1	3
47	Microkinetic Modeling of Surface Catalysis **2020**, 1377-1404		3
46	Reversible Formation of Silanol Groups in Two-Dimensional Siliceous Nanomaterials under Mild Hydrothermal Conditions. *Journal of Physical Chemistry C*, **2020**, 124, 18045-18053	3.8	3
45	Improved slit-shaped microseparator and its integration with a microreactor for modular biomanufacturing. *Green Chemistry*, **2021**, 23, 3700-3714	10	3
44	Synthesis of (hemi)cellulosic lubricant base oils via catalytic coupling and deoxygenation pathways. *Green Chemistry*, **2021**, 23, 4916-4930	10	3
43	Accurate Thermochemistry of Complex Lignin Structures via Density Functional Theory, Group Additivity, and Machine Learning. *ACS Sustainable Chemistry and Engineering*, **2021**, 9, 3043-3049	8.3	3
42	Regularized machine learning on molecular graph model explains systematic error in DFT enthalpies. *Scientific Reports*, **2021**, 11, 14372	4.9	3
41	Microwave heating of slurries. *Chemical Engineering Journal*, **2021**, 417, 127892	14.7	3
40	Cost and energy efficient cyclic separation of 5-hydroxymethyl furfural from an aqueous solution. *Green Chemistry*, **2021**, 23, 4008-4023	10	3
39	Programmable heating and quenching for efficient thermochemical synthesis.. *Nature*, **2022**, 605, 470-476	50.4	3

38	Phosphonate-Modified UiO-66 Brønsted Acid Catalyst and Its Use in Dehydra-Decyclization of 2-Methyltetrahydrofuran to Pentadienes. *Angewandte Chemie*, **2020**, 132, 13362-13368	3.6	2
37	Molecular valves actuated by intermolecular forces. *Physical Review E*, **2005**, 71, 060201	2.4	2
36	Reaction network reduction for distributed systems by model training in lumped reactors: Application to bifurcations in combustion. *Chaos*, **1999**, 9, 95-107	3.3	2
35	Modular Plasma Microreactor for Intensified Hydrogen Peroxide Production. *ACS Sustainable Chemistry and Engineering*, **2022**, 10, 1829-1838	8.3	2
34	Accelerating manufacturing for biomass conversion via integrated process and bench digitalization: a perspective. *Reaction Chemistry and Engineering*,	4.9	2
33	Inline Rolling Shear Alignment: Deposition and Long-Range Order of Block Polymer Templates in a Fast, Single-Step Process. *ACS Applied Polymer Materials*,	4.3	2
32	Lignin monomer conversion into biolubricant base oils. *Green Chemistry*, **2021**, 23, 10090-10100	10	2
31	Thermochemical Data Fusion Using Graph Representation Learning. *Journal of Chemical Information and Modeling*, **2020**, 60, 4673-4683	6.1	2
30	Experimental data-driven reaction network identification and uncertainty quantification of CO2-assisted ethane dehydrogenation over Ga2O3/Al2O3. *Chemical Engineering Science*, **2021**, 237, 116534	4.4	2
29	Experimental and Theoretical Insights into the Active Sites on WOx/Pt(111) Surfaces for Dehydrogenation and Dehydration Reactions. *ACS Catalysis*, **2021**, 11, 8023-8032	13.1	2
28	Scaling of Transition State Vibrational Frequencies and Application of d-Band Theory to the Brønsted–Evans–Polanyi Relationship on Surfaces. *Journal of Physical Chemistry C*, **2021**, 125, 7119-7129	3.8	2
27	Catalytic Hydrotreatment of Humins to Bio-Oil in Methanol over Supported Metal Catalysts. *ChemSusChem*, **2018**, 11, 3545-3545	8.3	2
26	Chemical Kinetics Bayesian Inference Toolbox (CKBIT). *Computer Physics Communications*, **2021**, 265, 107989	4.2	2
25	Production of renewable oleo-furan surfactants by cross-ketonization of biomass-derived furoic acid and fatty acids. *Catalysis Science and Technology*, **2021**, 11, 2762-2769	5.5	2
24	110th Anniversary: Kinetics and X-ray Absorption Spectroscopy in Methane Total Oxidation over Alumina-Supported Pt, Pd, and AgPd Catalysts. *Industrial & Engineering Chemistry Research*, **2019**, 58, 17718-17726	3.9	1
23	Transport Phenomena in Microscale Reacting Flows **2013**, 283-302		1
22	Microreactor Engineering: Processes, Detailed Design and Modeling179-198		1
21	Kinetics of Facet Formation During Growth and Etching of Crystals. *Materials Research Society Symposia Proceedings*, **1991**, 237, 145		1

20	Brønsted Acid Catalysis of the Direct Acylation of 2-Methylfuran by Acetic Acid. Theoretical Insights into the Role of Brønsted Acidity and Confinement. *ACS Catalysis*, **2021**, 11, 9916-9925	13.1	1
19	Microkinetic Modeling of Surface Catalysis **2018**, 1-28		1
18	Learning Chemistry of Complex Reaction Systems via a Python First-Principles Reaction Rule Stencil (pReSt) Generator. *Journal of Chemical Information and Modeling*, **2021**, 61, 3431-3441	6.1	1
17	Real-time dynamics and structures of supported subnanometer catalysts via multiscale simulations. *Nature Communications*, **2021**, 12, 5430	17.4	1
16	Prediction of Transition-State Scaling Relationships and Universal Transition-State Vibrational and Entropic Correlations for Dehydrogenations. *Journal of Physical Chemistry C*, **2021**, 125, 19780-19790	3.8	1
15	Mathematical Strategies for the Coarse-Graining of Microscopic Models **2005**, 1477-1490		1
14	Plasma technology for lignocellulosic biomass conversion toward an electrified biorefinery. *Green Chemistry*, **2022**, 24, 2680-2721	10	1
13	Microwave Heating-Induced Temperature Gradients in Liquid–Liquid Biphasic Systems. *Industrial & Engineering Chemistry Research*, **2022**, 61, 3011-3022	3.9	1
12	Automated exploitation of the big configuration space of large adsorbates on transition metals reveals chemistry feasibility.. *Nature Communications*, **2022**, 13, 2087	17.4	1
11	Python Group Additivity (pGrAdd) software for estimating species thermochemical properties. *Computer Physics Communications*, **2022**, 273, 108277	4.2	0
10	Uncertainty Quantification and Error Propagation in the Enthalpy and Entropy of Surface Reactions Arising from a Single DFT Functional. *Journal of Physical Chemistry C*, **2021**, 125, 18187-18196	3.8	0
9	Volcano curves for homologous series reactions: Oxidation of small alkanes. *Applied Catalysis A: General*, **2019**, 587, 117255	5.1	
8	Branched Bio-Lubricant Base Oil Production through Aldol Condensation. *ChemSusChem*, **2019**, 12, 47238.3		
7	Catalytic Hydrodeoxygenation of High Carbon Furylmethanes to Renewable Jet-fuel Ranged Alkanes over a Rhenium-Modified Iridium Catalyst. *ChemSusChem*, **2017**, 10, 3164-3164	8.3	
6	The role of reaction engineering in cancer biology: Bio-imaging informatics reveals implications of the plasma membrane heterogeneities. *Chemical Engineering Science*, **2007**, 62, 5222-5231	4.4	
5	Mesoscopic modeling of binary diffusion through microporous zeolite membranes. *Materials Research Society Symposia Proceedings*, **2002**, 752, 1		
4	Continuum and Stochastic Modeling on the Role of Gel Microstructure in Zeolite Crystallization. *Materials Research Society Symposia Proceedings*, **1996**, 431, 197		
3	Mathematical Strategies for the Coarse-Graining of Microscopic Models **2005**, 1477-1490		

2 Ozone Treatment **2005**, 1993-2001

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