Dionisios G Vlachos

List of Publications by Year in Descending Order

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	Ambient-pressure lignin valorization to high-performance polymers by intensified reductive catalytic deconstruction.. *Science Advances*, **2022**, 8, eabj7523	14.3	4
432	Catalytic resonance of ammonia synthesis by simulated dynamic ruthenium crystal strain.. *Science Advances*, **2022**, 8, eabl6576	14.3	3
431	Modular Plasma Microreactor for Intensified Hydrogen Peroxide Production. *ACS Sustainable Chemistry and Engineering*, **2022**, 10, 1829-1838	8.3	2
430	Python Group Additivity (pGrAdd) software for estimating species thermochemical properties. *Computer Physics Communications*, **2022**, 273, 108277	4.2	0
429	Intensified reactive extraction for the acid-catalyzed conversion of fructose to 5-hydroxymethyl furfural. *Chemical Engineering Journal*, **2022**, 428, 132556	14.7	5
428	Plasma technology for lignocellulosic biomass conversion toward an electrified biorefinery. *Green Chemistry*, **2022**, 24, 2680-2721	10	1
427	Modulating the dynamics of Br□sted acid sites on PtWOx inverse catalyst. *Nature Catalysis*, **2022**, 5, 144-153	36.5	5
426	Microwave Heating-Induced Temperature Gradients in Liquid□liquid Biphasic Systems. *Industrial & Engineering Chemistry Research*, **2022**, 61, 3011-3022	3.9	1
425	Automated exploitation of the big configuration space of large adsorbates on transition metals reveals chemistry feasibility.. *Nature Communications*, **2022**, 13, 2087	17.4	1
424	Programmable heating and quenching for efficient thermochemical synthesis.. *Nature*, **2022**, 605, 470-476	50.4	3
423	Lignin monomer conversion into biolubricant base oils. *Green Chemistry*, **2021**, 23, 10090-10100	10	2
422	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
421	A Review of Microwave-assisted Process Intensified Multiphase Reactors. *Chemical Engineering Journal*, **2021**, 133183	14.7	5
420	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
419	Process Systems Engineering Perspective on the Design of Materials and Molecules. *Industrial & Engineering Chemistry Research*, **2021**, 60, 5194-5206	3.9	11
418	Plastic waste to fuels by hydrocracking at mild conditions. *Science Advances*, **2021**, 7,	14.3	53
417	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

416	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
415	Polypropylene Plastic Waste Conversion to Lubricants over Ru/TiO2 Catalysts. *ACS Catalysis*, **2021**, 11, 8104-8115	13.1	22
414	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
413	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
412	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
411	One-step lignocellulose depolymerization and saccharification to high sugar yield and less condensed isolated lignin. *Green Chemistry*, **2021**, 23, 1200-1211	10	8
410	Fast microflow kinetics and acid catalyst deactivation in glucose conversion to 5-hydroxymethylfurfural. *Reaction Chemistry and Engineering*, **2021**, 6, 152-164	4.9	9
409	Improved slit-shaped microseparator and its integration with a microreactor for modular biomanufacturing. *Green Chemistry*, **2021**, 23, 3700-3714	10	3
408	Ethane Dehydrogenation on Single and Dual Centers of Ga-modified γ-Al2O3. *ACS Catalysis*, **2021**, 11, 1380-1391	13.1	10
407	A review of thermal and thermocatalytic valorization of food waste. *Green Chemistry*, **2021**, 23, 2806-2833	10	10
406	Synthesis of (hemi)cellulosic lubricant base oils via catalytic coupling and deoxygenation pathways. *Green Chemistry*, **2021**, 23, 4916-4930	10	3
405	Liquid–liquid Microfluidic Flows for Ultrafast 5-Hydroxymethyl Furfural Extraction. *Industrial & Engineering Chemistry Research*, **2021**, 60, 3723-3735	3.9	11
404	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
403	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
402	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
401	Regularized machine learning on molecular graph model explains systematic error in DFT enthalpies. *Scientific Reports*, **2021**, 11, 14372	4.9	3
400	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
399	Chemical Kinetics Bayesian Inference Toolbox (CKBIT). *Computer Physics Communications*, **2021**, 265, 107989	4.2	2

398	Microwave heating of slurries. *Chemical Engineering Journal*, **2021**, 417, 127892	14.7	3
397	Recent Advances in the Photocatalytic Conversion of Biomass-Derived Furanic Compounds. *ACS Catalysis*, **2021**, 11, 11336-11359	13.1	20
396	Polyethylene Hydrogenolysis at Mild Conditions over Ruthenium on Tungstated Zirconia. *Jacs Au*, **2021**, 1, 1422-1434		15
395	Ethylene production by direct conversion of methane over isolated single active centers. *Chemical Engineering Journal*, **2021**, 420, 130493	14.7	7
394	Real-time dynamics and structures of supported subnanometer catalysts via multiscale simulations. *Nature Communications*, **2021**, 12, 5430	17.4	1
393	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
392	Intensified microwave-assisted heterogeneous catalytic reactors for sustainable chemical manufacturing. *Chemical Engineering Journal*, **2021**, 420, 130476	14.7	5
391	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
390	Cost and energy efficient cyclic separation of 5-hydroxymethyl furfural from an aqueous solution. *Green Chemistry*, **2021**, 23, 4008-4023	10	3
389	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
388	Temperature Homogeneity under Selective and Localized Microwave Heating in Structured Flow Reactors. *Industrial & Engineering Chemistry Research*, **2021**, 60, 6835-6847	3.9	7
387	The Future is Garbage: Repurposing of Food Waste to an Integrated Biorefinery. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 8124-8136	8.3	20
386	Operation and Optimization of Microwave-Heated Continuous-Flow Microfluidics. *Industrial & Engineering Chemistry Research*, **2020**, 59, 10418-10427	3.9	8
385	Phosphonate-Modified UiO-66 Brønsted Acid Catalyst and Its Use in Dehydra-Decyclization of 2-Methyltetrahydrofuran to Pentadienes. *Angewandte Chemie - International Edition*, **2020**, 59, 13260-13266	16.4	9
384	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
383	Multiscale modeling of microwave-heated multiphase systems. *Chemical Engineering Journal*, **2020**, 397, 125262	14.7	7
382	Reaction Network Viewer (ReNView): An open-source framework for reaction path visualization of chemical reaction systems. *SoftwareX*, **2020**, 11, 100442	2.7	4
381	Infrared spectroscopy data- and physics-driven machine learning for characterizing surface microstructure of complex materials. *Nature Communications*, **2020**, 11, 1513	17.4	30

380	C□O bond activation using ultralow loading of noble metal catalysts on moderately reducible oxides. *Nature Catalysis*, **2020**, 3, 446-453	36.5	62
379	Growth kinetics of humins studied via X-ray scattering. *Green Chemistry*, **2020**, 22, 2301-2309	10	9
378	Catalytic resonance theory: parallel reaction pathway control. *Chemical Science*, **2020**, 11, 3501-3510	9.4	12
377	Understanding solvent effects on adsorption and protonation in porous catalysts. *Nature Communications*, **2020**, 11, 1060	17.4	38
376	Microkinetic Modeling of Surface Catalysis **2020**, 1377-1404		3
375	Thermochemical Data Fusion Using Graph Representation Learning. *Journal of Chemical Information and Modeling*, **2020**, 60, 4673-4683	6.1	2
374	Experiments and computations of microfluidic liquid□liquid flow patterns. *Reaction Chemistry and Engineering*, **2020**, 5, 39-50	4.9	22
373	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
372	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
371	Surface chemistry dictates stability and oxidation state of supported single metal catalyst atoms. *Chemical Science*, **2020**, 11, 1469-1477	9.4	8
370	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
369	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
368	Stability of heterogeneous single-atom catalysts: a scaling law mapping thermodynamics to kinetics. *Npj Computational Materials*, **2020**, 6,	10.9	17
367	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
366	Finite-Temperature Structures of Supported Subnanometer Catalysts Inferred Statistical Learning and Genetic Algorithm-Based Optimization. *ACS Nano*, **2020**, 14, 13995-14007	16.7	8
365	Explainable and trustworthy artificial intelligence for correctable modeling in chemical sciences. *Science Advances*, **2020**, 6,	14.3	12
364	Spectroscopic Probe Molecule Selection Using Quantum Theory, First-Principles Calculations, and Machine Learning. *ACS Nano*, **2020**,	16.7	4
363	Solvent selection for biphasic extraction of 5-hydroxymethylfurfural via multiscale modeling and experiments. *Green Chemistry*, **2020**, 22, 8699-8712	10	11

362	Active learning-driven quantitative synthesis–structure–property 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
361	The Catalytic Mechanics of Dynamic Surfaces: Stimulating Methods for Promoting Catalytic Resonance. *ACS Catalysis*, **2020**, 10, 12666-12695	13.1	18
360	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
359	Scaleup of a Single-Mode Microwave Reactor. *Industrial & Engineering Chemistry Research*, **2020**, 59, 2516-2523	3.9	14
358	A Python Multiscale Thermochemistry Toolbox (pMuTT) for thermochemical and kinetic parameter estimation. *Computer Physics Communications*, **2020**, 247, 106864	4.2	21
357	110th Anniversary: Kinetics and X-ray Absorption Spectroscopy in Methane Total Oxidation over Alumina-Supported Pt, Pd, and Ag–Pd Catalysts. *Industrial & Engineering Chemistry Research*, **2019**, 58, 17718-17726	3.9	1
356	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
355	Volcano curves for homologous series reactions: Oxidation of small alkanes. *Applied Catalysis A: General*, **2019**, 587, 117255	5.1	
354	Dehydra-Decyclization of Tetrahydrofuran on H-ZSM5: Mechanisms, Pathways, and Transition State Entropy. *ACS Catalysis*, **2019**, 9, 10279-10293	13.1	16
353	Renewable lubricants with tailored molecular architecture. *Science Advances*, **2019**, 5, eaav5487	14.3	30
352	Ultrafast flow chemistry for the acid-catalyzed conversion of fructose. *Energy and Environmental Science*, **2019**, 12, 2463-2475	35.4	28
351	Catalytic production of renewable lubricant base oils from bio-based 2-alkylfurans and enals. *Green Chemistry*, **2019**, 21, 3606-3614	10	17
350	First-Principles Kinetic and Spectroscopic Insights into Single-Atom Catalysis. *ACS Catalysis*, **2019**, 9, 5002-5010	13.1	24
349	Theoretical Approach To Predict the Stability of Supported Single-Atom Catalysts. *ACS Catalysis*, **2019**, 9, 3289-3297	13.1	59
348	Optimization of the facet structure of transition-metal catalysts applied to the oxygen reduction reaction. *Nature Chemistry*, **2019**, 11, 449-456	17.6	39
347	Fundamentals of C–O bond activation on metal oxide catalysts. *Nature Catalysis*, **2019**, 2, 269-276	36.5	46
346	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
345	Homogeneous Metal Salt Solutions for Biomass Upgrading and Other Select Organic Reactions. *ACS Catalysis*, **2019**, 9, 9923-9952	13.1	33

344	Lattice Convolutional Neural Network Modeling of Adsorbate Coverage Effects. *Journal of Physical Chemistry C*, **2019**, 123, 18951-18959	3.8	16
343	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
342	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
341	Branched Bio-Lubricant Base Oil Production through Aldol Condensation. *ChemSusChem*, **2019**, 12, 4780-4785	8.3	13
340	Branched Bio-Lubricant Base Oil Production through Aldol Condensation. *ChemSusChem*, **2019**, 12, 4723-	8.3	
339	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
338	Multiscale Modeling Combined with Active Learning for Microstructure Optimization of Bifunctional Catalysts. *Industrial & Engineering Chemistry Research*, **2019**, 58, 6146-6154	3.9	9
337	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
336	Microkinetic modeling of aqueous phase biomass conversion: Application to ethylene glycol reforming. *Chemical Engineering Science*, **2019**, 197, 415-418	4.4	9
335	Thermochemistry of gas-phase and surface species via LASSO-assisted subgraph selection. *Reaction Chemistry and Engineering*, **2018**, 3, 454-466	4.9	22
334	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
333	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
332	Structural analysis of humins formed in the Brønsted acid catalyzed dehydration of fructose. *Green Chemistry*, **2018**, 20, 997-1006	10	85
331	Oxidation of aromatic oxygenates for the production of terephthalic acid. *Applied Catalysis A: General*, **2018**, 552, 98-104	5.1	6
330	Non-parametric correlative uncertainty quantification and sensitivity analysis: Application to a Langmuir bimolecular adsorption model. *AIP Advances*, **2018**, 8, 035021	1.5	6
329	Mechanistic Study of the Direct Hydrodeoxygenation of m-Cresol over WOx-Decorated Pt/C Catalysts. *ACS Catalysis*, **2018**, 8, 7749-7759	13.1	58
328	Acylation of methylfuran with Brønsted and Lewis acid zeolites. *Applied Catalysis A: General*, **2018**, 564, 90-101	5.1	27
327	Cooperative Catalysis by Surface Lewis Acid/Silanol for Selective Fructose Etherification on Sn-SPP Zeolite. *ACS Catalysis*, **2018**, 8, 9056-9065	13.1	9

326	Spectroscopic characterization of a highly selective NiCu3/C hydrodeoxygenation catalyst. *Catalysis Science and Technology*, **2018**, 8, 6100-6108	5.5	9
325	Microkinetic Modeling of Surface Catalysis **2018**, 1-28		1
324	Kinetic Studies of Acid Hydrolysis of Food Waste-Derived Saccharides. *Industrial & Engineering Chemistry Research*, **2018**, 57, 17365-17374	3.9	10
323	Recent advances in understanding the pH dependence of the hydrogen oxidation and evolution reactions. *Journal of Catalysis*, **2018**, 367, 328-331	7.3	22
322	Catalytic Hydrotreatment of Humins to Bio-Oil in Methanol over Supported Metal Catalysts. *ChemSusChem*, **2018**, 11, 3545-3545	8.3	2
321	Catalytic Hydrotreatment of Humins to Bio-Oil in Methanol over Supported Metal Catalysts. *ChemSusChem*, **2018**, 11, 3609-3617	8.3	10
320	Direct speciation methods to quantify catalytically active species of AlCl in glucose isomerization.. *RSC Advances*, **2018**, 8, 17101-17109	3.7	17
319	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
318	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
317	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
316	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
315	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
314	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
313	Biomass-Derived Butadiene by Dehydra-Decyclization of Tetrahydrofuran. *ACS Sustainable Chemistry and Engineering*, **2017**, 5, 3732-3736	8.3	67
312	Distribution of open sites in Sn-Beta zeolite. *Microporous and Mesoporous Materials*, **2017**, 245, 45-50	5.3	25
311	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
310	Nanoporous Cu□□Co Alloys for Selective Furfural Hydrodeoxygenation to 2-Methylfuran. *Industrial & Engineering Chemistry Research*, **2017**, 56, 3866-3872	3.9	25
309	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

308	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
307	Selective hydrodeoxygenation of tartaric acid to succinic acid. *Catalysis Science and Technology*, **2017**, 7, 4944-4954	5.5	12
306	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
305	Group Additivity for Aqueous Phase Thermochemical Properties of Alcohols on Pt(111). *Journal of Physical Chemistry C*, **2017**, 121, 21510-21519	3.8	25
304	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
303	Durable and self-hydrating tungsten carbide-based composite polymer electrolyte membrane fuel cells. *Nature Communications*, **2017**, 8, 418	17.4	33
302	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
301	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
300	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	
299	Scaling relationships and theory for vibrational frequencies of adsorbates on transition metal surfaces. *Nature Communications*, **2017**, 8, 1842	17.4	16
298	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
297	1,2-H- versus 1,2-C-Shift on Sn-Silsesquioxanes. *ACS Catalysis*, **2017**, 7, 25-33	13.1	7
296	Diels–Alder cycloaddition of 2-methylfuran and ethylene for renewable toluene. *Applied Catalysis B: Environmental*, **2016**, 180, 487-496	21.8	70
295	Adsorption in zeolites using mechanically embedded ONIOM clusters. *Physical Chemistry Chemical Physics*, **2016**, 18, 26094-26106	3.6	32
294	Group Additivity for Thermochemical Property Estimation of Lignin Monomers on Pt(111). *Journal of Physical Chemistry C*, **2016**, 120, 19234-19241	3.8	14
293	Tunable Oleo-Furan Surfactants by Acylation of Renewable Furans. *ACS Central Science*, **2016**, 2, 820-824	16.8	41
292	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
291	Nickel supported on nitrogen-doped carbon nanotubes as hydrogen oxidation reaction catalyst in alkaline electrolyte. *Nature Communications*, **2016**, 7, 10141	17.4	269

290	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
289	Effects of correlated parameters and uncertainty in electronic-structure-based chemical kinetic modelling. *Nature Chemistry*, **2016**, 8, 331-7	17.6	99
288	Inhibition of Xylene Isomerization in the Production of Renewable Aromatic Chemicals from Biomass-Derived Furans. *ACS Catalysis*, **2016**, 6, 2076-2088	13.1	19
287	Mechanistic Insights into Lewis Acid Metal Salt-Catalyzed Glucose Chemistry in Aqueous Solution. *ACS Catalysis*, **2016**, 6, 1497-1504	13.1	62
286	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
285	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
284	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
283	Molecular structure, morphology and growth mechanisms and rates of 5-hydroxymethyl furfural (HMF) derived humins. *Green Chemistry*, **2016**, 18, 1983-1993	10	201
282	Stochastic averaging and sensitivity analysis for two scale reaction networks. *Journal of Chemical Physics*, **2016**, 144, 074104	3.9	8
281	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
280	Mechanism of Dehydration of Phenols on Noble Metals via First-Principles Microkinetic Modeling. *ACS Catalysis*, **2016**, 6, 3047-3055	13.1	59
279	Mechanisms for High Selectivity in the Hydrodeoxygenation of 5-Hydroxymethylfurfural over PtCo Nanocrystals. *ACS Catalysis*, **2016**, 6, 4095-4104	13.1	100
278	Pt catalysts for efficient aerobic oxidation of glucose to glucaric acid in water. *Green Chemistry*, **2016**, 18, 3815-3822	10	64
277	Reaction Pathways and Intermediates in Selective Ring Opening of Biomass-Derived Heterocyclic Compounds by Iridium. *ACS Catalysis*, **2016**, 6, 7002-7009	13.1	26
276	Insights into the Ring-Opening of Biomass-Derived Furanics over Carbon-Supported Ruthenium. *ChemSusChem*, **2016**, 9, 3113-3121	8.3	22
275	Methyl-ligated tin silsesquioxane catalyzed reactions of glucose. *Journal of Catalysis*, **2016**, 341, 62-71	7.3	12
274	Ring Activation of Furanic Compounds on Ruthenium-Based Catalysts. *Journal of Physical Chemistry C*, **2015**, 119, 6075-6085	3.8	25
273	Tandem Lewis/Brønsted 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

272	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
271	Building large microkinetic models with first-principles? accuracy at reduced computational cost. *Chemical Engineering Science*, **2015**, 121, 190-199	4.4	52
270	Reaction Pathways of Biomass-Derived Oxygenates over Metals and Carbides: From Model Surfaces to Supported Catalysts. *ChemCatChem*, **2015**, 7, 1402-1421	5.2	42
269	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
268	Mechanism of Br□sted Acid-Catalyzed Glucose Dehydration. *ChemSusChem*, **2015**, 8, 1291-1291	8.3	3
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