Alexei A Lapkin

List of Publications by Year
in descending order

134	6,260	71102	79698
papers	citations	41 h-index	73 g-index

160	160	160	7172
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Multi-objective Bayesian optimisation of a two-step synthesis of p-cymene from crude sulphate turpentine. Chemical Engineering Science, 2022, 247, 116938.	3.8	15
2	From Platform to Knowledge Graph: Evolution of Laboratory Automation. Jacs Au, 2022, 2, 292-309.	7.9	42
3	Efficient surrogates construction of chemical processes: Case studies on pressure swing adsorption and <scp>gasâ€toâ€liquids</scp>. AICHE Journal, 2022, 68, .	3.6	1
4	Minor Product Polymerization Causes Failure of High-Current CO₂-to-Ethylene Electrolyzers. ACS Energy Letters, 2022, 7, 599-601.	17.4	10
5	Accelerating net zero from the perspective of optimizing a carbon capture and utilization system. Energy and Environmental Science, 2022, 15, 2139-2153.	30.8	24
6	The effect of chemical representation on active machine learning towards closed-loop optimization. Reaction Chemistry and Engineering, 2022, 7, 1368-1379.	3.7	20
7	A review of molecular representation in the age of machine learning. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	14.6	75
8	Designing the process designer: Hierarchical reinforcement learning for optimisation-based process design. Chemical Engineering and Processing: Process Intensification, 2022, 180, 108885.	3.6	9
9	Discovering Circular Process Solutions through Automated Reaction Network Optimization. ACS Engineering Au, 2022, 2, 333-349.	5.1	1
10	Summit: Benchmarking Machine Learning Methods for Reaction Optimisation. Chemistry Methods, 2021, 1, 116-122.	3.8	34
11	Teaching sustainability as complex systems approach: a sustainable development goals workshop. International Journal of Sustainability in Higher Education, 2021, 22, 25-41.	3.1	19
12	Investigating CO₂ Methanation on Ni and Ru: DFT Assisted Microkinetic Analysis. ChemCatChem, 2021, 13, 2420-2433.	3.7	19
13	Carbon neutral manufacturing via on-site CO2 recycling. IScience, 2021, 24, 102514.	4.1	29
14	Efficient Syntheses of Biobased Terephthalic Acid, p-Toluic Acid, and p-Methylacetophenone via One-Pot Catalytic Aerobic Oxidation of Monoterpene Derived Bio-p-cymene. ACS Sustainable Chemistry and Engineering, 2021, 9, 8642-8652.	6.7	12
15	Active Learning Training Strategy for Predicting O Adsorption Free Energy on Perovskite Catalysts using Inexpensive Catalyst Features. Chemistry Methods, 2021, 1, 444-450.	3.8	2
16	Efficient hybrid multiobjective optimization of pressure swing adsorption. Chemical Engineering Journal, 2021, 423, 130248.	12.7	20
17	Pushing nanomaterials up to the kilogram scale â€“ An accelerated approach for synthesizing antimicrobial ZnO with high shear reactors, machine learning and high-throughput analysis. Chemical Engineering Journal, 2021, 426, 131345.	12.7	15
18	Chemical data intelligence for sustainable chemistry. Chemical Society Reviews, 2021, 50, 12013-12036.	38.1	21

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19	Economically viable CO₂ electroreduction embedded within ethylene oxide manufacturing. Energy and Environmental Science, 2021, 14, 1530-1543.	30.8	24
20	Optimization of Formulations Using Robotic Experiments Driven by Machine Learning DoE. Cell Reports Physical Science, 2021, 2, 100295.	5.6	28
21	Assembly of Two-Dimensional Metal Organic Framework Superstructures via Solvent-Mediated Oriented Attachment. Journal of Physical Chemistry C, 2021, 125, 22837-22847.	3.1	7
22	Techno-economic assessment of emerging CO2 electrolysis technologies. STAR Protocols, 2021, 2, 100889.	1.2	11
23	A Machine Learningâ€Enabled Autonomous Flow Chemistry Platform for Process Optimization of Multiple Reaction Metrics. Chemistry Methods, 2021, 1, 71-77.	3.8	25
24	Transition to sustainable chemistry through digitalization. CheM, 2021, 7, 2866-2882.	11.7	39
25	Rational Design of Continuous Flow Processes for Synthesis of Functional Molecules. , 2020, , 415-433.		1
26	A new formulation for symbolic regression to identify physico-chemical laws from experimental data. Chemical Engineering Journal, 2020, 387, 123412.	12.7	27
27	Automated self-optimisation of multi-step reaction and separation processes using machine learning. Chemical Engineering Journal, 2020, 384, 123340.	12.7	97
28	Hydrogen production of solar-driven steam gasification of sewage sludge in an indirectly irradiated fluidized-bed reactor. Applied Energy, 2020, 261, 114229.	10.1	31
29	Machine Learning-aided Process Design for Formulated Products. Computer Aided Chemical Engineering, 2020, 48, 1789-1794.	0.5	4
30	Modelling Circular Structures in Reaction Networks: Petri Nets and Reaction Network Flux Analysis. Computer Aided Chemical Engineering, 2020, , 1843-1848.	0.5	4
31	Searching for optimal process routes: A reinforcement learning approach. Computers and Chemical Engineering, 2020, 141, 107027.	3.8	23
32	Introduction to green chemistry and reaction engineering. Reaction Chemistry and Engineering, 2020, 5, 2131-2133.	3.7	7
33	Solvent Selection for Mitsunobu Reaction Driven by an Active Learning Surrogate Model. Organic Process Research and Development, 2020, 24, 2864-2873.	2.7	12
34	Investigating methane dry reforming on Ni and B promoted Ni surfaces: DFT assisted microkinetic analysis and addressing the coking problem. Catalysis Science and Technology, 2020, 10, 6628-6643.	4.1	23
35	Stochastic data-driven model predictive control using gaussian processes. Computers and Chemical Engineering, 2020, 139, 106844.	3.8	66
36	The role of NO2 and NO in the mechanism of hydrocarbon degradation leading to carbonaceous deposits in engines. Fuel, 2020, 267, 117218.	6.4	7

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37	In silico rationalisation of selectivity and reactivity in Pd-catalysed Câ€“H activation reactions. Beilstein Journal of Organic Chemistry, 2020, 16, 1465-1475.	2.2	2
38	Scalable and precise synthesis of two-dimensional metal organic framework nanosheets in a high shear annular microreactor. Chemical Engineering Journal, 2020, 388, 124133.	12.7	17
39	Identification of strategic molecules for future circular supply chains using large reaction networks. Reaction Chemistry and Engineering, 2019, 4, 1969-1981.	3.7	16
40	Towards circular economy: integration of bio-waste into chemical supply chain. Current Opinion in Chemical Engineering, 2019, 26, 148-156.	7.8	35
41	Machine learning and molecular descriptors enable rational solvent selection in asymmetric catalysis. Chemical Science, 2019, 10, 6697-6706.	7.4	84
42	Biosynthesis of spathulenol and camphor stand as a competitive route to artemisinin production as revealed by a new chemometric convergence approach based on nine locationsâ€™ field-grown Artemesia annua L.. Industrial Crops and Products, 2019, 137, 521-527.	5.2	3
43	Box-Behnken design based CO2 co-gasification of horticultural waste and sewage sludge with addition of ash from waste as catalyst. Applied Energy, 2019, 242, 1549-1561.	10.1	25
44	Nonlinear model predictive control with explicit back-offs for Gaussian process state space models. , 2019, , .		5
45	Heterogeneous benzaldehyde nitration in batch and continuous flow microreactor. Chemical Engineering Journal, 2019, 377, 120346.	12.7	21
46	Review of advanced physical and dataâ€driven models for dynamic bioprocess simulation: Case study of algaeâ€“bacteria consortium wastewater treatment. Biotechnology and Bioengineering, 2019, 116, 342-353.	3.3	33
47	Synergistic Contribution of the Acidic Metal Oxideâ€“Metal Couple and Solvent Environment in the Selective Hydrogenolysis of Glycerol: A Combined Experimental and Computational Study Using ReO_xâ€“Ir as the Catalyst. ACS Catalysis, 2019, 9, 485-503.	11.2	40
48	Continuous synthesis of doped layered double hydroxides in a meso-scale flow reactor. Chemical Engineering Journal, 2019, 360, 190-199.	12.7	17
49	Efficient multiobjective optimization employing Gaussian processes, spectral sampling and a genetic algorithm. Journal of Global Optimization, 2018, 71, 407-438.	1.8	153
50	Interpretation of the Vibrational Spectra of Glassy Polymers Using Coarse-Grained Simulations. Macromolecules, 2018, 51, 1559-1572.	4.8	25
51	Statistics of the network of organic chemistry. Reaction Chemistry and Engineering, 2018, 3, 102-118.	3.7	34
52	The concept of selectivity control by simultaneous distribution of the oxygen feed and wall temperature in a microstructured reactor. Chemical Engineering Journal, 2018, 331, 765-776.	12.7	6
53	The need for innovation management and decision guidance in sustainable process design. Journal of Cleaner Production, 2018, 172, 2374-2388.	9.3	22
54	Stochastic Nonlinear Model Predictive Control Using Gaussian Processes. , 2018, , .		22

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55	Nitrogen Removal and Energy Recovery from Sewage Sludge by Combined Hydrothermal Pretreatment and CO₂ Gasification. ACS Sustainable Chemistry and Engineering, 2018, 6, 16629-16636.	6.7	20
56	Hydrodynamic assembly of two-dimensional layered double hydroxide nanostructures. Nature Communications, 2018, 9, 4913.	12.8	38
57	Chemical storage of renewable energy. Science, 2018, 360, 707-708.	12.6	150
58	Machine learning meets continuous flow chemistry: Automated optimization towards the Pareto front of multiple objectives. Chemical Engineering Journal, 2018, 352, 277-282.	12.7	221
59	Borate-assisted liquid-phase selective oxidation of n-pentane. Applied Catalysis A: General, 2018, 563, 28-42.	4.3	6
60	Dynamic modeling and optimization of sustainable algal production with uncertainty using multivariate Gaussian processes. Computers and Chemical Engineering, 2018, 118, 143-158.	3.8	47
61	Porous Nanocrystalline Silicon Supported Bimetallic Pd-Au Catalysts: Preparation, Characterization, and Direct Hydrogen Peroxide Synthesis. Frontiers in Chemistry, 2018, 6, 85.	3.6	32
62	Improved stability of Y2O3 supported Ni catalysts for CO2 methanation by precursor-determined metal-support interaction. Applied Catalysis B: Environmental, 2018, 237, 504-512.	20.2	99
63	Intensification of Nitrobenzaldehydes Synthesis from Benzyl Alcohol in a Microreactor. Organic Process Research and Development, 2017, 21, 357-364.	2.7	14
64	A possible extension to the RInChI as a means of providing machine readable process data. Journal of Cheminformatics, 2017, 9, 23.	6.1	7
65	Direct valorisation of waste cocoa butter triglycerides via catalytic epoxidation, ringâ€opening and polymerisation. Journal of Chemical Technology and Biotechnology, 2017, 92, 2254-2266.	3.2	12
66	Automation of route identification and optimisation based on data-mining and chemical intuition. Faraday Discussions, 2017, 202, 483-496.	3.2	23
67	A Multiobjective Optimization Including Results of Life Cycle Assessment in Developing Biorenewablesâ€Based Processes. ChemSusChem, 2017, 10, 3632-3643.	6.8	31
68	Towards automation of chemical process route selection based on data mining. Green Chemistry, 2017, 19, 140-152.	9.0	26
69	Self-optimisation and model-based design of experiments for developing a Câ€“H activation flow process. Beilstein Journal of Organic Chemistry, 2017, 13, 150-163.	2.2	70
70	Continuousâ€Flow Synthesis and Derivatization of Aziridines through Palladiumâ€Catalyzed C(sp³)â^'H Activation. Angewandte Chemie, 2016, 128, 9024-9029.	2.0	10
71	Continuousâ€Flow Synthesis and Derivatization of Aziridines through Palladiumâ€Catalyzed C(sp³)â^'H Activation. Angewandte Chemie - International Edition, 2016, 55, 8878-8883.	13.8	55
72	Feasibility of Using 2,3,3,3-Tetrafluoropropene (R1234yf) as a Solvent for Solidâ€“Liquid Extraction of Biopharmaceuticals. ACS Sustainable Chemistry and Engineering, 2016, 4, 2559-2568.	6.7	12

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73	Continuous flow Buchwaldâ€“Hartwig amination of a pharmaceutical intermediate. Reaction Chemistry and Engineering, 2016, 1, 229-238.	3.7	38
74	A Continuous Process for Buchwaldâ€“Hartwig Amination at Micro-, Lab-, and Mesoscale Using a Novel Reactor Concept. Organic Process Research and Development, 2016, 20, 558-567.	2.7	48
75	Microtomography-based numerical simulations of heat transfer and fluid flow through Î² -SiC open-cell foams for catalysis. Catalysis Today, 2016, 278, 350-360.	4.4	50
76	Multivariate data analysis and metabolic profiling of artemisinin and related compounds in high yielding varieties of Artemisia annua field-grown in Madagascar. Journal of Pharmaceutical and Biomedical Analysis, 2016, 117, 522-531.	2.8	18
77	Pd/C catalysts based on synthetic carbons with bi- and tri-modal pore-size distribution: applications in flow chemistry. Catalysis Science and Technology, 2016, 6, 2387-2395.	4.1	10
78	Continuous Flow Metathesis for Direct Valorization of Food Waste: An Example of Cocoa Butter Triglyceride. ACS Sustainable Chemistry and Engineering, 2015, 3, 1453-1459.	6.7	29
79	Feasibility of the Simultaneous Determination of Monomer Concentrations and Particle Size in Emulsion Polymerization Using in Situ Raman Spectroscopy. Industrial & Engineering Chemistry Research, 2015, 54, 12867-12876.	3.7	19
80	Automatic discovery and optimization of chemical processes. Current Opinion in Chemical Engineering, 2015, 9, 1-7.	7.8	92
81	Closed-Loop Multitarget Optimization for Discovery of New Emulsion Polymerization Recipes. Organic Process Research and Development, 2015, 19, 1049-1053.	2.7	43
82	Selective telomerisation of isoprene with methanol by a heterogeneous palladium resin catalyst. Catalysis Science and Technology, 2015, 5, 1206-1212.	4.1	10
83	Synthesis of the antimalarial API artemether in a flow reactor. Catalysis Today, 2015, 239, 90-96.	4.4	19
84	Heterogenization of Pdâ€“NHC complexes onto a silica support and their application in Suzukiâ€“Miyaura coupling under batch and continuous flow conditions. Catalysis Science and Technology, 2015, 5, 310-319.	4.1	58
85	Alternative methods of processing bio-feedstocks in formulated consumer product design. Frontiers in Chemistry, 2014, 2, 26.	3.6	1
86	Tandem isomerization/telomerization of long chain dienes. Frontiers in Chemistry, 2014, 2, 37.	3.6	3
87	Comparative Cytotoxicity of Artemisinin and Cisplatin and Their Interactions with Chlorogenic Acids in MCF7 Breast Cancer Cells. ChemMedChem, 2014, 9, 2791-2797.	3.2	58
88	Facile biocatalytic synthesis of a macrocyclic lactone in sub- and supercritical solvents. Biocatalysis and Biotransformation, 2014, 32, 125-131.	2.0	19
89	Optimization of a Scalable Photochemical Reactor for Reactions with Singlet Oxygen. Organic Process Research and Development, 2014, 18, 1443-1454.	2.7	60
90	Integrating medicinal plants extraction into a high-value biorefinery: An example of Artemisia annua L.. Comptes Rendus Chimie, 2014, 17, 232-241.	0.5	15

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91	Non-equilibrium dynamic control of gold nanoparticle and hyper-branched nanogold assemblies. Chemical Science, 2014, 5, 1153.	7.4	19
92	Combining Gaussian processes, mutual information and a genetic algorithm for multi-target optimization of expensive-to-evaluate functions. Engineering Optimization, 2014, 46, 1593-1607.	2.6	30
93	The effect of O-methylated flavonoids and other co-metabolites on the crystallization and purification of artemisinin. Journal of Biotechnology, 2014, 171, 25-33.	3.8	14
94	Efficient reduction of bromates using carbon nanofibre supported catalysts: Experimental and a comparative life cycle assessment study. Chemical Engineering Journal, 2014, 248, 230-241.	12.7	36
95	Poly(acrylates) via SET-LRP in a continuous tubular reactor. Polymer Chemistry, 2013, 4, 4809.	3.9	60
96	A rapid method for the determination of artemisinin and its biosynthetic precursors in Artemisia annua L. crude extracts. Journal of Pharmaceutical and Biomedical Analysis, 2013, 84, 269-277.	2.8	43
97	Pollution prevention in the pharmaceutical industry. International Journal of Sustainable Engineering, 2013, 6, 344-351.	3.5	7
98	Anti-Plasmodial Polyvalent Interactions in Artemisia annua L. Aqueous Extract â€“ Possible Synergistic and Resistance Mechanisms. PLoS ONE, 2013, 8, e80790.	2.5	70
99	Kinetic Modeling of Nitrate Reduction Catalyzed by Pdâ€“Cu Supported on Carbon Nanotubes. Industrial & Engineering Chemistry Research, 2012, 51, 4854-4860.	3.7	20
100	Facile Stoichiometric Reductions in Flow: An Example of Artemisinin. Organic Process Research and Development, 2012, 16, 1039-1042.	2.7	37
101	A conceptual framework for description of complexity in intensive chemical processes. Chemical Engineering and Processing: Process Intensification, 2011, 50, 1027-1034.	3.6	14
102	Copper-catalyzed rearrangement of oximes into primary amides. Tetrahedron Letters, 2011, 52, 4252-4255.	1.4	67
103	Screening of new solvents for artemisininextraction process using ab initio methodology. Green Chemistry, 2010, 12, 241-251.	9.0	64
104	In situ synthesis and catalytic activity in CO oxidation of metal nanoparticles supported on porous nanocrystalline silicon. Journal of Catalysis, 2010, 271, 59-66.	6.2	27
105	Synthesis of high aspect ratio titanate nanotubes. Journal of Materials Chemistry, 2010, 20, 6484.	6.7	74
106	Telomerisation of long-chain dienes with alcohols using Pd(IMes)(dvds) catalyst. Green Chemistry, 2010, 12, 866.	9.0	22
107	Coupling of Heck and hydrogenation reactions in a continuous compact reactor. Journal of Catalysis, 2009, 267, 114-120.	6.2	40
108	Rheological behaviour of ethylene glycol-titanate nanotube nanofluids. Journal of Nanoparticle Research, 2009, 11, 1513-1520.	1.9	136

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109	Hybrid metal/silicon nanocomposite systems and their catalytic activity. Physica Status Solidi C: Current Topics in Solid State Physics, 2009, 6, 1575-1579.	0.8	2
110	An iron-catalysed synthesis of amides from nitriles and amines. Tetrahedron Letters, 2009, 50, 4262-4264.	1.4	72
111	Rheological behaviour of nanofluids containing tube / rod-like nanoparticles. Powder Technology, 2009, 194, 132-141.	4.2	126
112	Development of HPLC analytical protocols for quantification of artemisinin in biomass and extracts. Journal of Pharmaceutical and Biomedical Analysis, 2009, 49, 908-915.	2.8	65
113	Liquid phase hydrogenation in a structured multichannel reactor. Catalysis Today, 2009, 147, S313-S318.	4.4	16
114	Energy Minimization of Single-Walled Titanium Oxide Nanotubes. ACS Nano, 2009, 3, 3401-3412.	14.6	19
115	CFD optimisation of up-flow vertical HVPE reactor for GaN growth. Journal of Crystal Growth, 2008, 310, 3358-3365.	1.5	17
116	Heat transfer and flow behaviour of aqueous suspensions of titanate nanotubes (nanofluids). Powder Technology, 2008, 183, 63-72.	4.2	234
117	Chemically surface-modified carbon nanoparticle carrier for phenolic pollutants: Extraction and electrochemical determination of benzophenone-3 and triclosan. Analytica Chimica Acta, 2008, 616, 28-35.	5.4	64
118	Synthesis and catalytic activity of hybrid metal/silicon nanocomposites. Physica Status Solidi - Rapid Research Letters, 2008, 2, 132-134.	2.4	19
119	Potential of â€˜nanofluidsâ€™ to further intensify microreactors. Green Chemistry, 2008, 10, 670.	9.0	54
120	Highly selective Pd/titanate nanotube catalysts for the double-bond migration reaction. Journal of Catalysis, 2007, 245, 272-278.	6.2	65
121	Forced convective heat transfer of nanofluids. Advanced Powder Technology, 2007, 18, 813-824.	4.1	132
122	The effect of adsorbent characteristics on the performance of a continuous sorption-enhanced steam methane reforming process. Chemical Engineering Science, 2007, 62, 5632-5637.	3.8	14
123	Stability of Aqueous Suspensions of Titanate Nanotubes. Chemistry of Materials, 2006, 18, 1124-1129.	6.7	160
124	Microcalorimetric Study of Ammonia Chemisorption on H3PW12O40Supported onto Mesoporous Synthetic Carbons and SBA-15. Langmuir, 2006, 22, 7664-7671.	3.5	11
125	Comparative Assessment of Technologies for Extraction of Artemisinin. Journal of Natural Products, 2006, 69, 1653-1664.	3.0	161
126	Deposition of Pt, Pd, Ru and Au on the surfaces of titanate nanotubes. Topics in Catalysis, 2006, 39, 151-160.	2.8	131

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127	Sustainability Performance Indicators. , 2006, , 39-53.		6
128	Selective oxidation of alcohols in a continuous multifunctional reactor: Ruthenium oxide catalysed oxidation of benzyl alcohol. Applied Catalysis A: General, 2005, 288, 175-184.	4.3	80
129	Liquid-Phase Oxidation of Organic Feedstock in a Compact Multichannel Reactor. Industrial & Engineering Chemistry Research, 2005, 44, 9683-9690.	3.7	23
130	Reversible Storage of Molecular Hydrogen by Sorption into Multilayered TiO2Nanotubes. Journal of Physical Chemistry B, 2005, 109, 19422-19427.	2.6	219
131	Apparent Two-Dimensional Behavior of TiO2Nanotubes Revealed by Light Absorption and Luminescence. Journal of Physical Chemistry B, 2005, 109, 8565-8569.	2.6	124
132	The effect of hydrothermal conditions on the mesoporous structure of TiO2 nanotubes. Journal of Materials Chemistry, 2004, 14, 3370.	6.7	673
133	Framework for Evaluating the â€œGreennessâ€•of Chemical Processes:Â Case Studies for a Novel VOC Recovery Technology. Environmental Science & Technology, 2004, 38, 5815-5823.	10.0	43
134	Preparation and characterisation of chemisorbents based on heteropolyacids supported on synthetic mesoporous carbons and silica. Catalysis Today, 2003, 81, 611-621.	4.4	79