Alexei A Lapkin

List of Publications by Year
in descending order

134 papers	6,260 citations	71102 41 h-index	79698 73 g-index
160 all docs	160 docs citations	160 times ranked	7172 citing authors

#	Article	IF	Citations
1	The effect of hydrothermal conditions on the mesoporous structure of TiO2 nanotubes. Journal of Materials Chemistry, 2004, 14, 3370.	6.7	673
2	Heat transfer and flow behaviour of aqueous suspensions of titanate nanotubes (nanofluids). Powder Technology, 2008, 183, 63-72.	4.2	234
3	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
4	Reversible Storage of Molecular Hydrogen by Sorption into Multilayered TiO2Nanotubes. Journal of Physical Chemistry B, 2005, 109, 19422-19427.	2.6	219
5	Comparative Assessment of Technologies for Extraction of Artemisinin. Journal of Natural Products, 2006, 69, 1653-1664.	3.0	161
6	Stability of Aqueous Suspensions of Titanate Nanotubes. Chemistry of Materials, 2006, 18, 1124-1129.	6.7	160
7	Efficient multiobjective optimization employing Gaussian processes, spectral sampling and a genetic algorithm. Journal of Global Optimization, 2018, 71, 407-438.	1.8	153
8	Chemical storage of renewable energy. Science, 2018, 360, 707-708.	12.6	150
9	Rheological behaviour of ethylene glycol-titanate nanotube nanofluids. Journal of Nanoparticle Research, 2009, 11, 1513-1520.	1.9	136
10	Forced convective heat transfer of nanofluids. Advanced Powder Technology, 2007, 18, 813-824.	4.1	132
11	Deposition of Pt, Pd, Ru and Au on the surfaces of titanate nanotubes. Topics in Catalysis, 2006, 39, 151-160.	2.8	131
12	Rheological behaviour of nanofluids containing tube / rod-like nanoparticles. Powder Technology, 2009, 194, 132-141.	4.2	126
13	Apparent Two-Dimensional Behavior of TiO2Nanotubes Revealed by Light Absorption and Luminescence. Journal of Physical Chemistry B, 2005, 109, 8565-8569.	2.6	124
14	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
15	Automated self-optimisation of multi-step reaction and separation processes using machine learning. Chemical Engineering Journal, 2020, 384, 123340.	12.7	97
16	Automatic discovery and optimization of chemical processes. Current Opinion in Chemical Engineering, 2015, 9, 1-7.	7.8	92
17	Machine learning and molecular descriptors enable rational solvent selection in asymmetric catalysis. Chemical Science, 2019, 10, 6697-6706.	7.4	84
18	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

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19	Preparation and characterisation of chemisorbents based on heteropolyacids supported on synthetic mesoporous carbons and silica. Catalysis Today, 2003, 81, 611-621.	4.4	79
20	A review of molecular representation in the age of machine learning. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	14.6	75
21	Synthesis of high aspect ratio titanate nanotubes. Journal of Materials Chemistry, 2010, 20, 6484.	6.7	74
22	An iron-catalysed synthesis of amides from nitriles and amines. Tetrahedron Letters, 2009, 50, 4262-4264.	1.4	72
23	Anti-Plasmodial Polyvalent Interactions in Artemisia annua L. Aqueous Extract â€“ Possible Synergistic and Resistance Mechanisms. PLoS ONE, 2013, 8, e80790.	2.5	70
24	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
25	Copper-catalyzed rearrangement of oximes into primary amides. Tetrahedron Letters, 2011, 52, 4252-4255.	1.4	67
26	Stochastic data-driven model predictive control using gaussian processes. Computers and Chemical Engineering, 2020, 139, 106844.	3.8	66
27	Highly selective Pd/titanate nanotube catalysts for the double-bond migration reaction. Journal of Catalysis, 2007, 245, 272-278.	6.2	65
28	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
29	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
30	Screening of new solvents for artemisininextraction process using ab initio methodology. Green Chemistry, 2010, 12, 241-251.	9.0	64
31	Poly(acrylates) via SET-LRP in a continuous tubular reactor. Polymer Chemistry, 2013, 4, 4809.	3.9	60
32	Optimization of a Scalable Photochemical Reactor for Reactions with Singlet Oxygen. Organic Process Research and Development, 2014, 18, 1443-1454.	2.7	60
33	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
34	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
35	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
36	Potential of â€˜nanofluidsâ€™ to further intensify microreactors. Green Chemistry, 2008, 10, 670.	9.0	54

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37	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
38	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
39	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
40	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
41	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
42	Closed-Loop Multitarget Optimization for Discovery of New Emulsion Polymerization Recipes. Organic Process Research and Development, 2015, 19, 1049-1053.	2.7	43
43	From Platform to Knowledge Graph: Evolution of Laboratory Automation. Jacs Au, 2022, 2, 292-309.	7.9	42
44	Coupling of Heck and hydrogenation reactions in a continuous compact reactor. Journal of Catalysis, 2009, 267, 114-120.	6.2	40
45	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_{<i>x</i>}â€“Ir as the Catalyst. ACS Catalysis, 2019, 9, 485-503.	11.2	40
46	Transition to sustainable chemistry through digitalization. CheM, 2021, 7, 2866-2882.	11.7	39
47	Continuous flow Buchwaldâ€“Hartwig amination of a pharmaceutical intermediate. Reaction Chemistry and Engineering, 2016, 1, 229-238.	3.7	38
48	Hydrodynamic assembly of two-dimensional layered double hydroxide nanostructures. Nature Communications, 2018, 9, 4913.	12.8	38
49	Facile Stoichiometric Reductions in Flow: An Example of Artemisinin. Organic Process Research and Development, 2012, 16, 1039-1042.	2.7	37
50	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
51	Towards circular economy: integration of bio-waste into chemical supply chain. Current Opinion in Chemical Engineering, 2019, 26, 148-156.	7.8	35
52	Statistics of the network of organic chemistry. Reaction Chemistry and Engineering, 2018, 3, 102-118.	3.7	34
53	Summit: Benchmarking Machine Learning Methods for Reaction Optimisation. Chemistry Methods, 2021, 1, 116-122.	3.8	34
54	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

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55	Porous Nanocrystalline Silicon Supported Bimetallic Pd-Au Catalysts: Preparation, Characterization, and Direct Hydrogen Peroxide Synthesis. Frontiers in Chemistry, 2018, 6, 85.	3.6	32
56	A Multiobjective Optimization Including Results of Life Cycle Assessment in Developing Biorenewablesâ€Based Processes. ChemSusChem, 2017, 10, 3632-3643.	6.8	31
57	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
58	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
59	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
60	Carbon neutral manufacturing via on-site CO2 recycling. IScience, 2021, 24, 102514.	4.1	29
61	Optimization of Formulations Using Robotic Experiments Driven by Machine Learning DoE. Cell Reports Physical Science, 2021, 2, 100295.	5.6	28
62	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
63	A new formulation for symbolic regression to identify physico-chemical laws from experimental data. Chemical Engineering Journal, 2020, 387, 123412.	12.7	27
64	Towards automation of chemical process route selection based on data mining. Green Chemistry, 2017, 19, 140-152.	9.0	26
65	Interpretation of the Vibrational Spectra of Glassy Polymers Using Coarse-Grained Simulations. Macromolecules, 2018, 51, 1559-1572.	4.8	25
66	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
67	A Machine Learningâ€Enabled Autonomous Flow Chemistry Platform for Process Optimization of Multiple Reaction Metrics. Chemistry Methods, 2021, 1, 71-77.	3.8	25
68	Economically viable CO₂ electroreduction embedded within ethylene oxide manufacturing. Energy and Environmental Science, 2021, 14, 1530-1543.	30.8	24
69	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
70	Liquid-Phase Oxidation of Organic Feedstock in a Compact Multichannel Reactor. Industrial & Engineering Chemistry Research, 2005, 44, 9683-9690.	3.7	23
71	Automation of route identification and optimisation based on data-mining and chemical intuition. Faraday Discussions, 2017, 202, 483-496.	3.2	23
72	Searching for optimal process routes: A reinforcement learning approach. Computers and Chemical Engineering, 2020, 141, 107027.	3.8	23

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73	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
74	Telomerisation of long-chain dienes with alcohols using Pd(IMes)(dvds) catalyst. Green Chemistry, 2010, 12, 866.	9.0	22
75	The need for innovation management and decision guidance in sustainable process design. Journal of Cleaner Production, 2018, 172, 2374-2388.	9.3	22
76	Stochastic Nonlinear Model Predictive Control Using Gaussian Processes. , 2018, , .		22
77	Heterogeneous benzaldehyde nitration in batch and continuous flow microreactor. Chemical Engineering Journal, 2019, 377, 120346.	12.7	21
78	Chemical data intelligence for sustainable chemistry. Chemical Society Reviews, 2021, 50, 12013-12036.	38.1	21
79	Kinetic Modeling of Nitrate Reduction Catalyzed by Pdâ€“Cu Supported on Carbon Nanotubes. Industrial & Engineering Chemistry Research, 2012, 51, 4854-4860.	3.7	20
80	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
81	Efficient hybrid multiobjective optimization of pressure swing adsorption. Chemical Engineering Journal, 2021, 423, 130248.	12.7	20
82	The effect of chemical representation on active machine learning towards closed-loop optimization. Reaction Chemistry and Engineering, 2022, 7, 1368-1379.	3.7	20
83	Synthesis and catalytic activity of hybrid metal/silicon nanocomposites. Physica Status Solidi - Rapid Research Letters, 2008, 2, 132-134.	2.4	19
84	Energy Minimization of Single-Walled Titanium Oxide Nanotubes. ACS Nano, 2009, 3, 3401-3412.	14.6	19
85	Facile biocatalytic synthesis of a macrocyclic lactone in sub- and supercritical solvents. Biocatalysis and Biotransformation, 2014, 32, 125-131.	2.0	19
86	Non-equilibrium dynamic control of gold nanoparticle and hyper-branched nanogold assemblies. Chemical Science, 2014, 5, 1153.	7.4	19
87	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
88	Synthesis of the antimalarial API artemether in a flow reactor. Catalysis Today, 2015, 239, 90-96.	4.4	19
89	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
90	Investigating CO₂ Methanation on Ni and Ru: DFT Assisted Microkinetic Analysis. ChemCatChem, 2021, 13, 2420-2433.	3.7	19

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91	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
92	CFD optimisation of up-flow vertical HVPE reactor for GaN growth. Journal of Crystal Growth, 2008, 310, 3358-3365.	1.5	17
93	Continuous synthesis of doped layered double hydroxides in a meso-scale flow reactor. Chemical Engineering Journal, 2019, 360, 190-199.	12.7	17
94	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
95	Liquid phase hydrogenation in a structured multichannel reactor. Catalysis Today, 2009, 147, S313-S318.	4.4	16
96	Identification of strategic molecules for future circular supply chains using large reaction networks. Reaction Chemistry and Engineering, 2019, 4, 1969-1981.	3.7	16
97	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
98	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
99	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
100	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
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	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
103	Intensification of Nitrobenzaldehydes Synthesis from Benzyl Alcohol in a Microreactor. Organic Process Research and Development, 2017, 21, 357-364.	2.7	14
104	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
105	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
106	Solvent Selection for Mitsunobu Reaction Driven by an Active Learning Surrogate Model. Organic Process Research and Development, 2020, 24, 2864-2873.	2.7	12
107	Efficient Syntheses of Biobased Terephthalic Acid, <i>p</i>-Toluic Acid, and <i>p</i>-Methylacetophenone via One-Pot Catalytic Aerobic Oxidation of Monoterpene Derived Bio-<i>p</i>-cymene. ACS Sustainable Chemistry and Engineering, 2021, 9, 8642-8652.	6.7	12
108	Microcalorimetric Study of Ammonia Chemisorption on H3PW12O40Supported onto Mesoporous Synthetic Carbons and SBA-15. Langmuir, 2006, 22, 7664-7671.	3.5	11

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109	Techno-economic assessment of emerging CO2 electrolysis technologies. STAR Protocols, 2021, 2, 100889.	1.2	11
110	Selective telomerisation of isoprene with methanol by a heterogeneous palladium resin catalyst. Catalysis Science and Technology, 2015, 5, 1206-1212.	4.1	10
111	Continuousâ€Flow Synthesis and Derivatization of Aziridines through Palladiumâ€Catalyzed C(sp³)â^’H Activation. Angewandte Chemie, 2016, 128, 9024-9029.	2.0	10
112	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
113	Minor Product Polymerization Causes Failure of High-Current CO₂-to-Ethylene Electrolyzers. ACS Energy Letters, 2022, 7, 599-601.	17.4	10
114	Designing the process designer: Hierarchical reinforcement learning for optimisation-based process design. Chemical Engineering and Processing: Process Intensification, 2022, 180, 108885.	3.6	9
115	Pollution prevention in the pharmaceutical industry. International Journal of Sustainable Engineering, 2013, 6, 344-351.	3.5	7
116	A possible extension to the RInChI as a means of providing machine readable process data. Journal of Cheminformatics, 2017, 9, 23.	6.1	7
117	Introduction to green chemistry and reaction engineering. Reaction Chemistry and Engineering, 2020, 5, 2131-2133.	3.7	7
118	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
119	Assembly of Two-Dimensional Metal Organic Framework Superstructures <i>via</i> Solvent-Mediated Oriented Attachment. Journal of Physical Chemistry C, 2021, 125, 22837-22847.	3.1	7
120	Sustainability Performance Indicators. , 2006, , 39-53.		6
121	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
122	Borate-assisted liquid-phase selective oxidation of n-pentane. Applied Catalysis A: General, 2018, 563, 28-42.	4.3	6
123	Nonlinear model predictive control with explicit back-offs for Gaussian process state space models. , 2019, , .		5
124	Machine Learning-aided Process Design for Formulated Products. Computer Aided Chemical Engineering, 2020, 48, 1789-1794.	0.5	4
125	Modelling Circular Structures in Reaction Networks: Petri Nets and Reaction Network Flux Analysis. Computer Aided Chemical Engineering, 2020, , 1843-1848.	0.5	4
126	Tandem isomerization/telomerization of long chain dienes. Frontiers in Chemistry, 2014, 2, 37.	3.6	3

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127	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
128	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
129	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
130	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
131	Alternative methods of processing bio-feedstocks in formulated consumer product design. Frontiers in Chemistry, 2014, 2, 26.	3.6	1
132	Rational Design of Continuous Flow Processes for Synthesis of Functional Molecules. , 2020, , 415-433.		1
133	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
134	Discovering Circular Process Solutions through Automated Reaction Network Optimization. ACS Engineering Au, 2022, 2, 333-349.	5.1	1