

# Lei Zhang

## List of Publications by Year in descending order

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95  
papers

1,819  
citations

236912

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315719

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98  
docs citations

98  
times ranked

1128  
citing authors

#	ARTICLE	IF	CITATIONS
1	A generic methodology for processing route synthesis and design based on superstructure optimization. <i>Computers and Chemical Engineering</i> , 2017, 106, 892-910.	3.8	109
2	An optimization model for carbon capture utilization and storage supply chain: A case study in Northeastern China. <i>Applied Energy</i> , 2018, 231, 194-206.	10.1	80
3	New Vistas in Chemical Product and Process Design. <i>Annual Review of Chemical and Biomolecular Engineering</i> , 2016, 7, 557-582.	6.8	76
4	Generic mathematical programming formulation and solution for computer-aided molecular design. <i>Computers and Chemical Engineering</i> , 2015, 78, 79-84.	3.8	60
5	Chemical product design – recent advances and perspectives. <i>Current Opinion in Chemical Engineering</i> , 2020, 27, 22-34.	7.8	60
6	A machine learning based computer-aided molecular design/screening methodology for fragrance molecules. <i>Computers and Chemical Engineering</i> , 2018, 115, 295-308.	3.8	58
7	OptCAMD: An optimization-based framework and tool for molecular and mixture product design. <i>Computers and Chemical Engineering</i> , 2019, 124, 285-301.	3.8	58
8	A grand model for chemical product design. <i>Computers and Chemical Engineering</i> , 2016, 91, 15-27.	3.8	56
9	Design and comparison of energy-saving double column and triple column reactive-extractive hybrid distillation processes for ternary multi-azeotrope dehydration. <i>Separation and Purification Technology</i> , 2021, 259, 118211.	7.9	48
10	Computer aided chemical product design – ProCAPD and tailor-made blended products. <i>Computers and Chemical Engineering</i> , 2018, 116, 37-55.	3.8	46
11	Multi-objective optimization for the deployment of carbon capture utilization and storage supply chain considering economic and environmental performance. <i>Journal of Cleaner Production</i> , 2020, 270, 122481.	9.3	44
12	Mixed-integer bilevel optimization for capacity planning with rational markets. <i>Computers and Chemical Engineering</i> , 2016, 86, 33-47.	3.8	40
13	Optimization-based approach for CO <sub>2</sub> utilization in carbon capture, utilization and storage supply chain. <i>Computers and Chemical Engineering</i> , 2020, 139, 106885.	3.8	39
14	An integrated framework for designing formulated products. <i>Computers and Chemical Engineering</i> , 2017, 107, 61-76.	3.8	36
15	Structured solid electrolyte interphase enable reversible Li electrodeposition in flame-retardant phosphate-based electrolyte. <i>Energy Storage Materials</i> , 2021, 42, 628-635.	18.0	34
16	Food Product Design: A Hybrid Machine Learning and Mechanistic Modeling Approach. <i>Industrial &amp; Engineering Chemistry Research</i> , 2019, 58, 16743-16752.	3.7	33
17	Advances in chemical product design. <i>Reviews in Chemical Engineering</i> , 2018, 34, 319-340.	4.4	32
18	Design and control of a novel side-stream extractive distillation column for separating methanol-toluene binary azeotrope with intermediate boiling entrainer. <i>Separation and Purification Technology</i> , 2020, 239, 116581.	7.9	32

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19	Optimization and eco-efficiency analysis of extractive distillation processes with different solvents for separating the ternary mixture embedding two azeotropes. Separation and Purification Technology, 2021, 269, 118763.	7.9	32
20	Computer-aided reaction solvent design based on transition state theory and COSMO-SAC. Chemical Engineering Science, 2019, 202, 300-317.	3.8	31
21	Conceptual design and techno-economic analysis for a coal-to-SNG/methanol polygeneration process in series and parallel reactors with integration of waste heat recovery. Energy Conversion and Management, 2020, 214, 112890.	9.2	31
22	Conceptual design of the triple-column extractive distillation processes with single entrainer and double entrainer for separating the N-hexane/acetone/chloroform ternary multi-azeotropic mixture. Chemical Engineering Science, 2021, 237, 116578.	3.8	31
23	Design and control analysis of the side-stream extractive distillation column with low concentration intermediate-boiling entrainer. Chemical Engineering Science, 2022, 247, 116915.	3.8	31
24	Machine learning-based atom contribution method for the prediction of surface charge density profiles and solvent design. AIChE Journal, 2021, 67, e17110.	3.6	30
25	A novel pinch-based method for process integration and optimization of Kalina cycle. Energy Conversion and Management, 2020, 209, 112630.	9.2	29
26	Computer-aided Framework for Design of Pure, Mixed and Blended Products. Computer Aided Chemical Engineering, 2015, 37, 2093-2098.	0.5	27
27	Risk management optimization framework for the optimal deployment of carbon capture and storage system under uncertainty. Renewable and Sustainable Energy Reviews, 2019, 113, 109280.	16.4	27
28	Sustainable product design: A life-cycle approach. Chemical Engineering Science, 2020, 217, 115508.	3.8	27
29	Heat pump assisted extractive distillation sequences with intermediate-boiling entrainer. Applied Thermal Engineering, 2021, 186, 116511.	6.0	26
30	Computer-aided molecular design of solvents for chemical separation processes. Current Opinion in Chemical Engineering, 2022, 35, 100732.	7.8	24
31	A Computer-Aided Methodology for Mixture-Blend Design. Applications to Tailor-Made Design of Surrogate Fuels. Industrial & Engineering Chemistry Research, 2018, 57, 7008-7020.	3.7	23
32	Computer-Aided Polymer Design: Integrating Group Contribution and Molecular Dynamics. Industrial & Engineering Chemistry Research, 2019, 58, 15542-15552.	3.7	22
33	Thermodynamic performance assessment of SOFC-RC-KC system for multiple waste heat recovery. Energy Conversion and Management, 2021, 245, 114579.	9.2	22
34	A grand product design model for crystallization solvent design. Computers and Chemical Engineering, 2020, 135, 106764.	3.8	21
35	Economic evaluation and environmental assessment of shale gas dehydration process. Journal of Cleaner Production, 2019, 232, 487-498.	9.3	20
36	Advanced exergy analysis for the solid oxide fuel cell system combined with a kinetic-based modeling pre-reformer. Energy Conversion and Management, 2021, 245, 114560.	9.2	20

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37	Heat-integrated water allocation network synthesis for industrial parks with sequential and simultaneous design. <i>Computers and Chemical Engineering</i> , 2018, 108, 408-424.	3.8	18
38	Design and eco-efficiency analysis of sustainable extractive distillation process combining preconcentration and solvent recovery functions for separating the tetrahydrofuran/ethanol/water ternary multi-azeotropic mixture. <i>Chemical Engineering Research and Design</i> , 2022, 159, 795-808.	5.6	18
39	Upgraded Graphical Method for the Synthesis of Direct Work Exchanger Networks. <i>Industrial &amp; Engineering Chemistry Research</i> , 2017, 56, 14304-14315.	3.7	17
40	Product design: Impact of government policy and consumer preference on company profit and corporate social responsibility. <i>Computers and Chemical Engineering</i> , 2018, 118, 118-131.	3.8	17
41	Design and comparison of conventional and side-stream extractive distillation sequences for separating the methanol-toluene binary azeotrope with intermediate boiling entrainer. <i>Computers and Chemical Engineering</i> , 2020, 143, 107115.	3.8	17
42	Integrated solvent-process design methodology based on COSMO-SAC and quantum mechanics for TMQ (2,2,4-trimethyl-1,2-H-dihydroquinoline) production. <i>Chemical Engineering Science</i> , 2020, 226, 115894.	3.8	14
43	Heat exchanger network synthesis integrated with flexibility and controllability. <i>Chinese Journal of Chemical Engineering</i> , 2019, 27, 1474-1484.	3.5	12
44	Synthesis of Flexible Heat Exchanger Networks Considering Gradually Accumulated Deposit and Cleaning Management. <i>Industrial &amp; Engineering Chemistry Research</i> , 2019, 58, 12124-12136.	3.7	12
45	Optimization-based framework for the synthesis of heat exchanger networks incorporating controllability. <i>Energy</i> , 2020, 208, 118292.	8.8	12
46	Superstructure-Based Simultaneous Optimization of a Heat Exchanger Network and a Compression-Absorption Cascade Refrigeration System for Heat Recovery. <i>Industrial &amp; Engineering Chemistry Research</i> , 2020, 59, 16017-16028.	3.7	12
47	A simultaneous optimization model for a heat-integrated syngas-to-methanol process with Kalina Cycle for waste heat recovery. <i>Energy</i> , 2021, 227, 120536.	8.8	12
48	Synthesis and design of sustainable integrated process, water treatment, and power generation networks. <i>Computers and Chemical Engineering</i> , 2020, 141, 107041.	3.8	11
49	Crystallization solvent design based on a new quantitative prediction model of crystal morphology. <i>AIChE Journal</i> , 2022, 68, e17499.	3.6	11
50	Applications of Shannon's Entropy Theory to Naphtha Pyrolysis Simulation. <i>Chemical Engineering and Technology</i> , 2012, 35, 281-286.	1.5	10
51	A Generic Methodology for Superstructure Optimization of Different Processing Networks. <i>Computer Aided Chemical Engineering</i> , 2016, , 685-690.	0.5	10
52	Direct work exchanger network synthesis of isothermal process based on improved transshipment model. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2017, 81, 295-304.	5.3	10
53	Computer-aided reaction solvent design considering inertness using group contribution-based reaction thermodynamic model. <i>Chemical Engineering Research and Design</i> , 2019, 152, 123-133.	5.6	10
54	Multiobjective Optimization of Interplant Heat Exchanger Networks Considering Utility Steam Supply and Various Locations of Interplant Steam Generation/Utilization. <i>Industrial &amp; Engineering Chemistry Research</i> , 2020, 59, 14433-14446.	3.7	10

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55	Odor prediction and aroma mixture design using machine learning model and molecular surface charge density profiles. <i>Chemical Engineering Science</i> , 2021, 245, 116947.	3.8	10
56	VPPD-Lab. <i>Computer Aided Chemical Engineering</i> , 2016, 39, 61-94.	0.5	9
57	Product design: Incorporating make-or-buy analysis and supplier selection. <i>Chemical Engineering Science</i> , 2019, 202, 357-372.	3.8	9
58	Optimization-Based Framework for Designing Dynamic Flexible Heat Exchanger Networks. <i>Industrial &amp; Engineering Chemistry Research</i> , 2019, 58, 6026-6041.	3.7	9
59	Integrated Computer-aided Framework for Sustainable Chemical Product Design and Evaluation. <i>Computer Aided Chemical Engineering</i> , 2016, 38, 2343-2348.	0.5	8
60	Heat Exchanger Network Synthesis Integrated with Compression-Driven Absorption Cascade Refrigeration System. <i>Processes</i> , 2020, 8, 210.	2.8	8
61	A surrogate-based optimization framework for simultaneous synthesis of chemical process and heat exchanger network. <i>Chemical Engineering Research and Design</i> , 2021, 170, 180-188.	5.6	8
62	Control of energy-efficient extractive distillation configurations for separating the methanol/toluene azeotrope with intermediate-boiling entrainer. <i>Chemical Engineering and Processing: Process Intensification</i> , 2020, 149, 107862.	3.6	7
63	A computational toolbox for molecular property prediction based on quantum mechanics and quantitative structure-property relationship. <i>Frontiers of Chemical Science and Engineering</i> , 0, , 1.	4.4	7
64	Interplant Heat Integration Method Involving Multiple Intermediate Fluid Circles and Agents: Single-Period and Multiperiod Designs. <i>Industrial &amp; Engineering Chemistry Research</i> , 2020, 59, 4698-4711.	3.7	6
65	Computer-Aided Molecular Design and Property Prediction. <i>Computer Aided Chemical Engineering</i> , 2016, 39, 153-196.	0.5	5
66	Economic Evaluation and Environmental Assessment of the Shale Gas Sweetening Process. <i>Chemical Engineering and Technology</i> , 2019, 42, 753-760.	1.5	5
67	An extended superstructure modeling method for simultaneous synthesis of direct work exchanger networks. <i>Chemical Engineering Research and Design</i> , 2019, 144, 258-271.	5.6	5
68	A thermo-economic multi-objective optimization model for simultaneous synthesis of heat exchanger networks including compressors. <i>Chemical Engineering Research and Design</i> , 2020, 153, 120-135.	5.6	5
69	Computer-Aided Design of a Perfluorinated Sulfonic Acid Proton Exchange Membrane Using Stochastic Optimization and Molecular Dynamic Method. <i>Industrial &amp; Engineering Chemistry Research</i> , 2021, 60, 18045-18057.	3.7	5
70	Multi-objective optimization of heat exchange network and thermodynamic cycles integrated system for cooling and power cogeneration. <i>Applied Energy</i> , 2022, 321, 119366.	10.1	5
71	Simultaneous Optimization of a Heat-Integrated Coal-to-SNG/MeOH Polygeneration Process Based on Rigorous Kinetic Models. <i>Industrial &amp; Engineering Chemistry Research</i> , 2020, 59, 22247-22257.	3.7	4
72	An upgraded superstructure-based model for simultaneous synthesis of direct work and heat exchanger networks. <i>Chemical Engineering Research and Design</i> , 2020, 159, 377-394.	5.6	4

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73	Automatic data-driven stoichiometry identification and kinetic modeling framework for homogeneous organic reactions. <i>AIChE Journal</i> , 2022, 68, .	3.6	4
74	<i>De novo</i> drug design framework based on mathematical programming method and deep learning model. <i>AIChE Journal</i> , 0, , .	3.6	4
75	Simulation and Optimization of Multi-period Steam Cracking Process. , 0, , .		3
76	ProCAPD – A Computer-Aided Model-Based Tool for Chemical Product Design and Analysis. <i>Computer Aided Chemical Engineering</i> , 2018, 44, 469-474.	0.5	3
77	Process evaluation and optimization of methanol production from shale gas based on kinetics modeling. <i>Journal of Cleaner Production</i> , 2020, 274, 123153.	9.3	3
78	Enhancing the lubricity of gas-to-liquid (GTL) paraffinic kerosene: impact of the additives on the physicochemical properties. <i>BMC Chemical Engineering</i> , 2020, 2, .	3.4	3
79	Simultaneous synthesis of sub and above-ambient heat exchanger networks including expansion process based on an enhanced superstructure model. <i>Chinese Journal of Chemical Engineering</i> , 2020, 28, 1344-1356.	3.5	3
80	Simultaneous Synthesis of Heat Exchanger Networks Considering Steam Supply and Various Steam Heater Locations. <i>Energies</i> , 2020, 13, 1467.	3.1	3
81	An enhanced superstructure-based model for work-integrated heat exchange network considering inter-stage multiple utilities optimization. <i>Computers and Chemical Engineering</i> , 2021, 152, 107388.	3.8	3
82	A Platform of Machine Learning-Based Next-Generation Property Estimation Methods for CAMD. <i>Computer Aided Chemical Engineering</i> , 2021, , 227-233.	0.5	3
83	RetroSynX: A retrosynthetic analysis framework using hybrid reaction templates and group contribution-based thermodynamic models. <i>Chemical Engineering Science</i> , 2022, 248, 117208.	3.8	3
84	Dynamic controllability comparison of different side-stream extractive distillation processes with intermediate boiling entrainer. <i>Separation and Purification Technology</i> , 2022, 286, 120475.	7.9	3
85	Simultaneous Synthesis of WHEN Based on Superstructure Modelling Considering Thermodynamic and Economic Factors. <i>Computer Aided Chemical Engineering</i> , 2018, 44, 1033-1038.	0.5	2
86	A Versatile Modeling Framework for Integrated Chemical Product Design. <i>Industrial &amp; Engineering Chemistry Research</i> , 2021, 60, 436-456.	3.7	2
87	Water networks synthesis for industrial parks respecting to unpredictable scenarios. <i>Computer Aided Chemical Engineering</i> , 2018, , 1021-1026.	0.5	1
88	QMaC: A Quantum Mechanics/Machine Learning-based Computational Tool for Chemical Product Design. <i>Computer Aided Chemical Engineering</i> , 2020, 48, 1807-1812.	0.5	1
89	Integrated machine learning framework for computer-aided chemical product design. , 2021, , 325-359.		1
90	Two-tier control structure design methodology applied to heat exchanger networks. <i>Chinese Journal of Chemical Engineering</i> , 2022, 47, 231-244.	3.5	1

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91	A multi-scale model of naphtha pyrolysis process. Computer Aided Chemical Engineering, 2012, 31, 120-124.	0.5	0
92	Synthesis of indirect work exchange networks considering both isothermal and adiabatic process together with exergy analysis. Chinese Journal of Chemical Engineering, 2018, 26, 1644-1652.	3.5	0
93	GC-COSMO based Reaction Solvent Design with New Kinetic Model using CAMD. Computer Aided Chemical Engineering, 2018, , 235-240.	0.5	0
94	A versatile modelling system for integrated chemical product design problems. Computer Aided Chemical Engineering, 2021, , 75-80.	0.5	0
95	Computer-Aided Solvent Design Integrated with a Machine Learning-based Atom Contribution Method. Computer Aided Chemical Engineering, 2021, , 69-74.	0.5	0