

Hanyu Gao

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/5432779/publications.pdf>

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16
papers

1,047
citations

840776

11
h-index

996975

15
g-index

16
all docs

16
docs citations

16
times ranked

1319
citing authors

#	ARTICLE	IF	CITATIONS
1	A robotic platform for flow synthesis of organic compounds informed by AI planning. <i>Science</i> , 2019, 365, .	12.6	548
2	Using Machine Learning To Predict Suitable Conditions for Organic Reactions. <i>ACS Central Science</i> , 2018, 4, 1465-1476.	11.3	245
3	Acceleration of Kinetic Monte Carlo Method for the Simulation of Free Radical Copolymerization through Scaling. <i>Industrial & Engineering Chemistry Research</i> , 2015, 54, 11975-11985.	3.7	40
4	On the modeling of number and weight average molecular weight of polymers. <i>Chemical Engineering Journal</i> , 2017, 327, 906-913.	12.7	33
5	Towards efficient discovery of green synthetic pathways with Monte Carlo tree search and reinforcement learning. <i>Chemical Science</i> , 2020, 11, 10959-10972.	7.4	31
6	Machine learning for design principles for single atom catalysts towards electrochemical reactions. <i>Journal of Materials Chemistry A</i> , 2022, 10, 15309-15331.	10.3	28
7	Automated Chemical Reaction Extraction from Scientific Literature. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 2035-2045.	5.4	26
8	Design of Copolymers Based on Sequence Distribution for a Targeted Molecular Weight and Conversion. <i>Macromolecular Theory and Simulations</i> , 2014, 23, 564-574.	1.4	22
9	Acceleration of kinetic monte carlo simulations of free radical copolymerization: A hybrid approach with scaling. <i>AIChE Journal</i> , 2017, 63, 4013-4021.	3.6	18
10	Application and comparison of derivative-free optimization algorithms to control and optimize free radical polymerization simulated using the kinetic Monte Carlo method. <i>Computers and Chemical Engineering</i> , 2018, 108, 268-275.	3.8	17
11	Artificial Intelligence for Computer-Aided Synthesis In Flow: Analysis and Selection of Reaction Components. <i>Frontiers in Chemical Engineering</i> , 2020, 2, .	2.7	16
12	Machine Learning and Data Science in Chemical Engineering. <i>Industrial & Engineering Chemistry Research</i> , 2022, 61, 8357-8358.	3.7	9
13	Combining retrosynthesis and mixed-integer optimization for minimizing the chemical inventory needed to realize a WHO essential medicines list. <i>Reaction Chemistry and Engineering</i> , 2020, 5, 367-376.	3.7	5
14	Direct Optimization across Computer-Generated Reaction Networks Balances Materials Use and Feasibility of Synthesis Plans for Molecule Libraries. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 493-504.	5.4	5
15	A Combined Computational and Experimental Study of Copolymerization Propagation Kinetics for 1-Ethylcyclopentyl methacrylate and Methyl methacrylate. <i>Macromolecular Theory and Simulations</i> , 2016, 25, 263-273.	1.4	4
16	A Combined Computational and Experimental Study of Copolymerization Propagation Kinetics for 1-Ethylcyclopentyl methacrylate and Methyl methacrylate. <i>Macromolecular Theory and Simulations</i> , 2016, 25, 263-273.	1.4	0