Hanyu Gao

List of Publications by Year
in descending order

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