LoÃ¯c M Roch

List of Publications by Year
in descending order

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31 papers	2,202 citations	394421 19 h-index	434195 31 g-index
32 all docs	32 docs citations	32 times ranked	2877 citing authors

#	Article	IF	Citations
1	Accelerating the discovery of materials for clean energy in the era of smart automation. Nature Reviews Materials, 2018, 3, 5-20.	48.7	489
2	Self-driving laboratory for accelerated discovery of thin-film materials. Science Advances, 2020, 6, eaaz8867.	10.3	306
3	Phoenics: A Bayesian Optimizer for Chemistry. ACS Central Science, 2018, 4, 1134-1145.	11.3	215
4	Next-Generation Experimentation with Self-Driving Laboratories. Trends in Chemistry, 2019, 1, 282-291.	8.5	175
5	Beyond Ternary OPV: Highâ€Throughput Experimentation and Selfâ€Driving Laboratories Optimize Multicomponent Systems. Advanced Materials, 2020, 32, e1907801.	21.0	138
6	ChemOS: Orchestrating autonomous experimentation. Science Robotics, 2018, 3, .	17.6	113
7	Data-science driven autonomous process optimization. Communications Chemistry, 2021, 4, .	4.5	94
8	Chimera: enabling hierarchy based multi-objective optimization for self-driving laboratories. Chemical Science, 2018, 9, 7642-7655.	7.4	86
9	ChemOS: An orchestration software to democratize autonomous discovery. PLoS ONE, 2020, 15, e0229862.	2.5	77
10	A Bayesian Approach to Predict Solubility Parameters. Advanced Theory and Simulations, 2019, 2, 1800069.	2.8	62
11	G<scp>ryffin</scp>: An algorithm for Bayesian optimization of categorical variables informed by expert knowledge. Applied Physics Reviews, 2021, 8, .	11.3	61
12	Designing and understanding light-harvesting devices with machine learning. Nature Communications, 2020, 11, 4587.	12.8	57
13	Pentaindenocorannulene: Properties, Assemblies, and C₆₀ Complex. Angewandte Chemie - International Edition, 2016, 55, 14648-14652.	13.8	44
14	Interface Molecular Engineering for Laminated Monolithic Perovskite/Silicon Tandem Solar Cells with 80.4% Fill Factor. Advanced Functional Materials, 2019, 29, 1901476.	14.9	43
15	Olympus: a benchmarking framework for noisy optimization and experiment planning. Machine Learning: Science and Technology, 2021, 2, 035021.	5.0	31
16	Toward Accurate Adsorption Energetics on Clay Surfaces. Journal of Physical Chemistry C, 2016, 120, 26402-26413.	3.1	30
17	Kinetics of the Regeneration by Iodide of Dye Sensitizers Adsorbed on Mesoporous Titania. Journal of Physical Chemistry C, 2014, 118, 17108-17115.	3.1	26
18	Pentaindenocorannulene: Properties, Assemblies, and C₆₀ Complex. Angewandte Chemie, 2016, 128, 14868-14872.	2.0	25

#	Article	IF	Citations
19	General optimization procedure towards the design of a new family of minimal parameter spin-component-scaled double-hybrid density functional theory. Physical Chemistry Chemical Physics, 2017, 19, 26191-26200.	2.8	20
20	[3+3] Cyclocondensation of Disubstituted Biphenyl Dialdehydes: Access to Inherently Luminescent and Optically Active Hexa-substituted C₃-Symmetric and Asymmetric Trianglimine Macrocycles. Journal of Organic Chemistry, 2017, 82, 2472-2480.	3.2	19
21	Indenocorannulene-Based Materials: Effect of Solid-State Packing and Intermolecular Interactions on Optoelectronic Properties. Journal of Physical Chemistry C, 2017, 121, 1220-1234.	3.1	17
22	Azaindenocorannulenes: Synthesis, Properties, and Chirality. Organic Letters, 2019, 21, 3510-3513.	4.6	13
23	1,2,3- versus 1,2-Indeno Ring Fusions Influence Structure Property and Chirality of Corannulene Bowls. Journal of Organic Chemistry, 2018, 83, 3979-3986.	3.2	12
24	From Absorption Spectra to Charge Transfer in Nanoaggregates of Oligomers with Machine Learning. ACS Nano, 2020, 14, 6589-6598.	14.6	12
25	Diindenocorannulenes: Curved Aromatics Blending Bowlâ€inâ€Bowl Assembly and Nanocarbon Material Properties. European Journal of Organic Chemistry, 2017, 2017, 2801-2805.	2.4	11
26	Dispersion-Corrected Spin-Component-Scaled Double-Hybrid Density Functional Theory: Implementation and Performance for Non-covalent Interactions. Journal of Chemical Theory and Computation, 2017, 13, 2650-2666.	5.3	8
27	Melatonin-directed micellization: a case for tryptophan metabolites and their classical bioisosteres as templates for the self-assembly of bipyridinium-based supramolecular amphiphiles in water. Soft Matter, 2018, 14, 2893-2905.	2.7	8
28	The influence of sorbitol doping on aggregation and electronic properties of PEDOT:PSS: a theoretical study. Machine Learning: Science and Technology, 2021, 2, 01LT01.	5.0	4
29	Performance analysis of openâ€source distributed file systems for practical largeâ€scale molecular ab initio, density functional theory, and GWâ€‰+â€‰BSE calculations. International Journal of Quantum Chemistry, 2018, 118, e25392.	2.0	2
30	Film Fabrication Techniques: Beyond Ternary OPV: Highâ€Throughput Experimentation and Selfâ€Driving Laboratories Optimize Multicomponent Systems (Adv. Mater. 14/2020). Advanced Materials, 2020, 32, 2070110.	21.0	2
31	From 4T to 2T solution processed silicon/perovskite tandems solar cells. , 0, , .		0