

Loïc M Roch

List of Publications by Year in descending order

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Version: 2024-02-01

31
papers

2,202
citations

394421

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434195

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all docs

32
docs citations

32
times ranked

2877
citing authors

#	ARTICLE	IF	CITATIONS
1	The influence of sorbitol doping on aggregation and electronic properties of PEDOT:PSS: a theoretical study. <i>Machine Learning: Science and Technology</i> , 2021, 2, 01LT01.	5.0	4
2	Olympus: a benchmarking framework for noisy optimization and experiment planning. <i>Machine Learning: Science and Technology</i> , 2021, 2, 035021.	5.0	31
3	Data-science driven autonomous process optimization. <i>Communications Chemistry</i> , 2021, 4, .	4.5	94
4	G<scp>ryffin</scp>: An algorithm for Bayesian optimization of categorical variables informed by expert knowledge. <i>Applied Physics Reviews</i> , 2021, 8, .	11.3	61
5	Designing and understanding light-harvesting devices with machine learning. <i>Nature Communications</i> , 2020, 11, 4587.	12.8	57
6	Self-driving laboratory for accelerated discovery of thin-film materials. <i>Science Advances</i> , 2020, 6, eaaz8867.	10.3	306
7	Beyond Ternary OPV: High-Throughput Experimentation and Self-Driving Laboratories Optimize Multicomponent Systems. <i>Advanced Materials</i> , 2020, 32, e1907801.	21.0	138
8	Film Fabrication Techniques: Beyond Ternary OPV: High-Throughput Experimentation and Self-Driving Laboratories Optimize Multicomponent Systems (<i>Adv. Mater.</i> 14/2020). <i>Advanced Materials</i> , 2020, 32, 2070110.	21.0	2
9	From Absorption Spectra to Charge Transfer in Nanoaggregates of Oligomers with Machine Learning. <i>ACS Nano</i> , 2020, 14, 6589-6598.	14.6	12
10	ChemOS: An orchestration software to democratize autonomous discovery. <i>PLoS ONE</i> , 2020, 15, e0229862.	2.5	77
11	Interface Molecular Engineering for Laminated Monolithic Perovskite/Silicon Tandem Solar Cells with 80.4% Fill Factor. <i>Advanced Functional Materials</i> , 2019, 29, 1901476.	14.9	43
12	Next-Generation Experimentation with Self-Driving Laboratories. <i>Trends in Chemistry</i> , 2019, 1, 282-291.	8.5	175
13	Azaindenocorannulenes: Synthesis, Properties, and Chirality. <i>Organic Letters</i> , 2019, 21, 3510-3513.	4.6	13
14	A Bayesian Approach to Predict Solubility Parameters. <i>Advanced Theory and Simulations</i> , 2019, 2, 1800069.	2.8	62
15	Accelerating the discovery of materials for clean energy in the era of smart automation. <i>Nature Reviews Materials</i> , 2018, 3, 5-20.	48.7	489
16	1,2,3- versus 1,2-Indeno Ring Fusions Influence Structure Property and Chirality of Corannulene Bowls. <i>Journal of Organic Chemistry</i> , 2018, 83, 3979-3986.	3.2	12
17	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. <i>Soft Matter</i> , 2018, 14, 2893-2905.	2.7	8
18	Performance analysis of open-source distributed file systems for practical large-scale molecular <i>ab initio</i> , <i>density functional theory</i> , and <i>GW+BSE</i> calculations. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25392.	2.0	2

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19	Chimera: enabling hierarchy based multi-objective optimization for self-driving laboratories. <i>Chemical Science</i> , 2018, 9, 7642-7655.	7.4	86
20	Phoenics: A Bayesian Optimizer for Chemistry. <i>ACS Central Science</i> , 2018, 4, 1134-1145.	11.3	215
21	ChemOS: Orchestrating autonomous experimentation. <i>Science Robotics</i> , 2018, 3, .	17.6	113
22	Indenocorannulene-Based Materials: Effect of Solid-State Packing and Intermolecular Interactions on Optoelectronic Properties. <i>Journal of Physical Chemistry C</i> , 2017, 121, 1220-1234.	3.1	17
23	[3+3] Cyclocondensation of Disubstituted Biphenyl Dialdehydes: Access to Inherently Luminescent and Optically Active Hexa-substituted C_{3h} -Symmetric and Asymmetric Trianglimine Macrocycles. <i>Journal of Organic Chemistry</i> , 2017, 82, 2472-2480.	3.2	19
24	Diindenocorannulenes: Curved Aromatics Blending Bowl-in-Bowl Assembly and Nanocarbon Material Properties. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 2801-2805.	2.4	11
25	Dispersion-Corrected Spin-Component-Scaled Double-Hybrid Density Functional Theory: Implementation and Performance for Non-covalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2650-2666.	5.3	8
26	General optimization procedure towards the design of a new family of minimal parameter spin-component-scaled double-hybrid density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 26191-26200.	2.8	20
27	Pentaindenocorannulene: Properties, Assemblies, and C_{60} Complex. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 14648-14652.	13.8	44
28	Pentaindenocorannulene: Properties, Assemblies, and C_{60} Complex. <i>Angewandte Chemie</i> , 2016, 128, 14868-14872.	2.0	25
29	Toward Accurate Adsorption Energetics on Clay Surfaces. <i>Journal of Physical Chemistry C</i> , 2016, 120, 26402-26413.	3.1	30
30	Kinetics of the Regeneration by Iodide of Dye Sensitizers Adsorbed on Mesoporous Titania. <i>Journal of Physical Chemistry C</i> , 2014, 118, 17108-17115.	3.1	26
31	From 4T to 2T solution processed silicon/perovskite tandems solar cells. , 0, , .		0