Benjamin Sanchez-Lengeling

List of Publications by Year
in descending order

18 papers	5,005 citations	567281 15 h-index	839539 18 g-index
32 all docs	32 docs citations	32 times ranked	5101 citing authors

#	Article	IF	Citations
1	Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules. ACS Central Science, 2018, 4, 268-276.	11.3	1,761
2	Inverse molecular design using machine learning: Generative models for matter engineering. Science, 2018, 361, 360-365.	12.6	1,055
3	Rational design of layered oxide materials for sodium-ion batteries. Science, 2020, 370, 708-711.	12.6	616
4	Molecular Sets (MOSES): A Benchmarking Platform for Molecular Generation Models. Frontiers in Pharmacology, 2020, 11, 565644.	3.5	266
5	Reinforced Adversarial Neural Computer for de Novo Molecular Design. Journal of Chemical Information and Modeling, 2018, 58, 1194-1204.	5.4	256
6	Inverse Design of Solid-State Materials via a Continuous Representation. Matter, 2019, 1, 1370-1384.	10.0	198
7	Inverse design of nanoporous crystalline reticular materials with deep generative models. Nature Machine Intelligence, 2021, 3, 76-86.	16.0	172
8	Design Principles and Top Non-Fullerene Acceptor Candidates for Organic Photovoltaics. Joule, 2017, 1, 857-870.	24.0	157
9	Materials Acceleration Platforms: On the way to autonomous experimentation. Current Opinion in Green and Sustainable Chemistry, 2020, 25, 100370.	5.9	67
10	A Bayesian Approach to Predict Solubility Parameters. Advanced Theory and Simulations, 2019, 2, 1800069.	2.8	62
11	A Mixed Quantum Chemistry/Machine Learning Approach for the Fast and Accurate Prediction of Biochemical Redox Potentials and Its Large-Scale Application to 315â€¯000 Redox Reactions. ACS Central Science, 2019, 5, 1199-1210.	11.3	61
12	Introducing a New Potential Figure of Merit for Evaluating Microstructure Stability in Photovoltaic Polymer-Fullerene Blends. Journal of Physical Chemistry C, 2017, 121, 18153-18161.	3.1	52
13	Quantum Chemical Approach to Estimating the Thermodynamics of Metabolic Reactions. Scientific Reports, 2014, 4, 7022.	3.3	34
14	A machine learning workflow for molecular analysis: application to melting points. Machine Learning: Science and Technology, 2020, 1, 025015.	5.0	23
15	Quantum chemistry reveals thermodynamic principles of redox biochemistry. PLoS Computational Biology, 2018, 14, e1006471.	3.2	22
16	Coronene derivatives for transparent organic photovoltaics through inverse materials design. Journal of Materials Chemistry C, 2021, 9, 1310-1317.	5.5	12
17	A thermodynamic atlas of carbon redox chemical space. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 32910-32918.	7.1	11
18	Learning More, with Less. ACS Central Science, 2017, 3, 275-277.	11.3	6