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