Benjamin J Bucior

List of Publications by Year
in descending order

11	1,042	933447 10	1281871 11
papers	citations	h-index	g-index

11	11	11	1069
all docs	docs citations	times ranked	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	Machine learning using host/guest energy histograms to predict adsorption in metalâ€“organic frameworks: Application to short alkanes and Xe/Kr mixtures. Journal of Chemical Physics, 2021, 155, 014701.	3.0	24
3	Process-level modelling and optimization to evaluate metalâ€“organic frameworks for post-combustion capture of CO₂. Molecular Systems Design and Engineering, 2020, 5, 1205-1218.	3.4	37
4	Computational screening, synthesis and testing of metalâ€“organic frameworks with a bithiazole linker for carbon dioxide capture and its green conversion into cyclic carbonates. Molecular Systems Design and Engineering, 2019, 4, 1000-1013.	3.4	24
5	Advances, Updates, and Analytics for the Computation-Ready, Experimental Metalâ€“Organic Framework Database: CoRE MOF 2019. Journal of Chemical & Engineering Data, 2019, 64, 5985-5998.	1.9	372
6	Prediction of hydrogen adsorption in nanoporous materials from the energy distribution of adsorption sites. Molecular Physics, 2019, 117, 3683-3694.	1.7	23
7	Identification Schemes for Metalâ€“Organic Frameworks To Enable Rapid Search and Cheminformatics Analysis. Crystal Growth and Design, 2019, 19, 6682-6697.	3.0	123
8	Energy-based descriptors to rapidly predict hydrogen storage in metalâ€“organic frameworks. Molecular Systems Design and Engineering, 2019, 4, 162-174.	3.4	179
9	Adsorption and Diffusion of Fluids in Defective Carbon Nanotubes: Insights from Molecular Simulations. Langmuir, 2017, 33, 11834-11844.	3.5	9
10	Porous Carbon Nanotube Membranes for Separation of H₂/CH₄ and CO₂/CH₄ Mixtures. Journal of Physical Chemistry C, 2012, 116, 25904-25910.	3.1	59
11	Using Mesoscopic Models to Design Strong and Tough Biomimetic Polymer Networks. Langmuir, 2011, 27, 13796-13805.	3.5	20