Jacob I Monroe

List of Publications by Year
in descending order

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15 papers	517 citations	840728 11 h-index	996954 15 g-index
15 all docs	15 docs citations	15 times ranked	733 citing authors

#	Article	IF	Citations
1	Evidence for Entropically Controlled Interfacial Hydration in Mesoporous Organosilicas. Journal of the American Chemical Society, 2022, 144, 1766-1777.	13.7	20
2	Learning Efficient, Collective Monte Carlo Moves with Variational Autoencoders. Journal of Chemical Theory and Computation, 2022, 18, 3622-3636.	5.3	9
3	Quantifying Polypeptoid Conformational Landscapes through Integrated Experiment and Simulation. Macromolecules, 2021, 54, 5011-5021.	4.8	9
4	Affinity of small-molecule solutes to hydrophobic, hydrophilic, and chemically patterned interfaces in aqueous solution. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	24
5	Extrapolation and interpolation strategies for efficiently estimating structural observables as a function of temperature and density. Journal of Chemical Physics, 2020, 153, 144101.	3.0	12
6	Water Structure and Properties at Hydrophilic and Hydrophobic Surfaces. Annual Review of Chemical and Biomolecular Engineering, 2020, 11, 523-557.	6.8	57
7	Performing solvation free energy calculations in LAMMPS using the decoupling approach. Journal of Computer-Aided Molecular Design, 2020, 34, 641-646.	2.9	10
8	Decoding signatures of structure, bulk thermodynamics, and solvation in three-body angle distributions of rigid water models. Journal of Chemical Physics, 2019, 151, 094501.	3.0	16
9	Best Practices for Foundations in Molecular Simulations [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 1, .	6.4	105
10	Surface chemical heterogeneity modulates silica surface hydration. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 2890-2895.	7.1	105
11	Computational discovery of chemically patterned surfaces that effect unique hydration water dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 8093-8098.	7.1	43
12	Unraveling Hydrophobic Interactions at the Molecular Scale Using Force Spectroscopy and Molecular Dynamics Simulations. ACS Nano, 2017, 11, 2586-2597.	14.6	37
13	Are AMBER Force Fields and Implicit Solvation Models Additive? A Folding Study with a Balanced Peptide Test Set. Journal of Chemical Theory and Computation, 2016, 12, 5631-5642.	5.3	26
14	Converging free energies of binding in cucurbit[7]uril and octa-acid hostâ€“guest systems from SAMPL4 using expanded ensemble simulations. Journal of Computer-Aided Molecular Design, 2014, 28, 401-415.	2.9	39
15	Investigating the mutation resistance of nonnucleoside inhibitors of HIV-RT using multiple microsecond atomistic simulations. Proteins: Structure, Function and Bioinformatics, 2014, 82, 130-144.	2.6	5