Harold W Hatch

List of Publications by Year
in descending order

26 papers	440 citations	759233 12 h-index	752698 20 g-index
26 all docs	26 docs citations	26 times ranked	505 citing authors

#	Article	IF	Citations
1	Comments on â€œMonte Carlo simulations for water adsorption in porous materials: Best practices and new insightsâ€• AIChE Journal, 2022, 68, .	3.6	1
2	Flat-histogram extrapolation as a useful tool in the age of big data. Molecular Simulation, 2021, 47, 395-407.	2.0	7
3	Dynamic arrest of adhesive hard rod dispersions. Soft Matter, 2020, 16, 1279-1286.	2.7	9
4	Parallel Prefetching for Canonical Ensemble Monte Carlo Simulations. Journal of Physical Chemistry A, 2020, 124, 7191-7198.	2.5	1
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	Computational Investigation of Correlations in Adsorbate Entropy for Pure-Silica Zeolite Adsorbents. Journal of Physical Chemistry C, 2020, 124, 16350-16361.	3.1	4
7	Improving the efficiency of Monte Carlo simulations of ions using expanded grand canonical ensembles. Journal of Chemical Physics, 2019, 151, 144109.	3.0	4
8	Designing molecular building blocks for the self-assembly of complex porous networks. Molecular Systems Design and Engineering, 2019, 4, 644-653.	3.4	10
9	Evaluating the Effects of Hinge Flexibility on the Solution Structure of Antibodies at Concentrated Conditions. Journal of Pharmaceutical Sciences, 2019, 108, 1663-1674.	3.3	10
10	Tabular Potentials for Monte Carlo Simulation of Supertoroids with Short-Range Interactions. Journal of Research of the National Institute of Standards and Technology, 2019, 124, 1-11.	1.2	0
11	FEASST: Free Energy and Advanced Sampling Simulation Toolkit. Journal of Research of the National Institute of Standards and Technology, 2018, 123, 1-3.	1.2	16
12	Monte Carlo simulation of cylinders with short-range attractions. AIP Advances, 2018, 8, 095210.	1.3	9
13	A methodology to calculate small-angle scattering profiles of macromolecular solutions from molecular simulations in the grand-canonical ensemble. Journal of Chemical Physics, 2018, 149, 084203.	3.0	2
14	Predicting structural properties of fluids by thermodynamic extrapolation. Journal of Chemical Physics, 2018, 148, 194105.	3.0	12
15	Assembly of three-dimensional binary superlattices from multi-flavored particles. Soft Matter, 2018, 14, 6303-6312.	2.7	15
16	Molecular dynamics simulation of trimer self-assembly under shear. Fluid Phase Equilibria, 2017, 440, 87-94.	2.5	8
17	Assembly of multi-flavored two-dimensional colloidal crystals. Soft Matter, 2017, 13, 5397-5408.	2.7	19
18	Communication: Predicting virial coefficients and alchemical transformations by extrapolating Mayer-sampling Monte Carlo simulations. Journal of Chemical Physics, 2017, 147, 231102.	3.0	9

#	Article	IF	Citations
19	Depletion-driven crystallization of cubic colloids sedimented on a surface. Journal of Chemical Physics, 2016, 144, 194902.	3.0	14
20	Self-assembly of trimer colloids: effect of shape and interaction range. Soft Matter, 2016, 12, 4170-4179.	2.7	22
21	Computational study of trimer self-assembly and fluid phase behavior. Journal of Chemical Physics, 2015, 142, 164901.	3.0	23
22	Computational Study of the Stability of the Miniprotein Trp-Cage, the GB1 Î²-Hairpin, and the AK16 Peptide, under Negative Pressure. Journal of Physical Chemistry B, 2014, 118, 7761-7769.	2.6	37
23	Molecular modeling of mechanical stresses on proteins in glassy matrices: Formalism. Journal of Chemical Physics, 2012, 137, 035103.	3.0	16
24	Assessing the thermodynamic signatures of hydrophobic hydration for several common water models. Journal of Chemical Physics, 2010, 132, 124504.	3.0	71
25	Chiral symmetry breaking in a microscopic model with asymmetric autocatalysis and inhibition. Journal of Chemical Physics, 2010, 133, 224502.	3.0	19
26	Natively Unfolded Protein Stability as a Coil-to-Globule Transition in Charge/Hydropathy Space. Journal of the American Chemical Society, 2008, 130, 9536-9542.	13.7	90