David F Hahn

List of Publications by Year
in descending order

13 papers	348 citations	1163117 8 h-index	1125743 13 g-index
17 all docs	17 docs citations	17 times ranked	366 citing authors

#	Article	IF	Citations
1	Pre-Exascale Computing of Proteinâ€“Ligand Binding Free Energies with Open Source Software for Drug Design. Journal of Chemical Information and Modeling, 2022, 62, 1172-1177.	5.4	22
2	Ensembler: A Simple Package for Fast Prototyping and Teaching Molecular Simulations. Journal of Chemical Information and Modeling, 2021, 61, 560-564.	5.4	4
3	A Benchmark of Electrostatic Method Performance in Relative Binding Free Energy Calculations. Journal of Chemical Information and Modeling, 2021, 61, 1048-1052.	5.4	12
4	Development and Benchmarking of Open Force Field v1.0.0â€”the Parsley Small-Molecule Force Field. Journal of Chemical Theory and Computation, 2021, 17, 6262-6280.	5.3	80
5	Expanded Ensemble Methods Can be Used to Accurately Predict Protein-Ligand Relative Binding Free Energies. Journal of Chemical Theory and Computation, 2021, 17, 6536-6547.	5.3	7
6	Systematic Optimization of a Fragment-Based Force Field against Experimental Pure-Liquid Properties Considering Large Compound Families: Application to Saturated Haloalkanes. Journal of Chemical Theory and Computation, 2020, 16, 7525-7555.	5.3	21
7	The Conveyor Belt Umbrella Sampling (CBUS) Scheme: Principle and Application to the Calculation of the Absolute Binding Free Energies of Alkali Cations to Crown Ethers. Journal of Chemical Theory and Computation, 2020, 16, 2474-2493.	5.3	1
8	Overcoming Orthogonal Barriers in Alchemical Free Energy Calculations: On the Relative Merits of Î»-Variations, Î»-Extrapolations, and Biasing. Journal of Chemical Theory and Computation, 2020, 16, 1630-1645.	5.3	20
9	Benchmark assessment of molecular geometries and energies from small molecule force fields. F1000Research, 2020, 9, 1390.	1.6	30
10	Best Practices for Alchemical Free Energy Calculations [Article v1.0]. Living Journal of Computational Molecular Science, 2020, 2, .	6.4	125
11	<scp>Vase</scp>â€<scp>Kite</scp> Equilibrium of Resorcin[4]arene Cavitands Investigated Using Molecular Dynamics Simulations with Ballâ€andâ€Stick Local Elevation Umbrella Sampling. Helvetica Chimica Acta, 2019, 102, e1900060.	1.6	3
12	Alchemical Free-Energy Calculations by Multiple-Replica Î»-Dynamics: The Conveyor Belt Thermodynamic Integration Scheme. Journal of Chemical Theory and Computation, 2019, 15, 2392-2419.	5.3	17
13	Best Practices for Alchemical Free Energy Calculations [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 2, .	6.4	3