

David F Hahn

List of Publications by Year in descending order

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Version: 2024-02-01

13
papers

348
citations

1163117

8
h-index

1125743

13
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17
all docs

17
docs citations

17
times ranked

366
citing authors

#	ARTICLE	IF	CITATIONS
1	Best Practices for Alchemical Free Energy Calculations [Article v1.0]. Living Journal of Computational Molecular Science, 2020, 2, .	6.4	125
2	Development and Benchmarking of Open Force Field v1.0.0—the Parsley Small-Molecule Force Field. Journal of Chemical Theory and Computation, 2021, 17, 6262-6280.	5.3	80
3	Benchmark assessment of molecular geometries and energies from small molecule force fields. F1000Research, 2020, 9, 1390.	1.6	30
4	Pre-Exascale Computing of Protein–Ligand Binding Free Energies with Open Source Software for Drug Design. Journal of Chemical Information and Modeling, 2022, 62, 1172-1177.	5.4	22
5	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
6	Overcoming Orthogonal Barriers in Alchemical Free Energy Calculations: On the Relative Merits of λ -Variations, λ -Extrapolations, and Biasing. Journal of Chemical Theory and Computation, 2020, 16, 1630-1645.	5.3	20
7	Alchemical Free-Energy Calculations by Multiple-Replica λ -Dynamics: The Conveyor Belt Thermodynamic Integration Scheme. Journal of Chemical Theory and Computation, 2019, 15, 2392-2419.	5.3	17
8	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
9	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
10	Ensembler: A Simple Package for Fast Prototyping and Teaching Molecular Simulations. Journal of Chemical Information and Modeling, 2021, 61, 560-564.	5.4	4
11	$\langle \text{Vase} \rangle$ – $\langle \text{Kite} \rangle$ Equilibrium of Resorcin[4]arene Cavitands Investigated Using Molecular Dynamics Simulations with Ball-and-Stick Local Elevation Umbrella Sampling. Helvetica Chimica Acta, 2019, 102, e1900060.	1.6	3
12	Best Practices for Alchemical Free Energy Calculations [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 2, .	6.4	3
13	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