Haochuan Chen

List of Publications by Year
in descending order

14	1,064	933447	1058476
papers	citations	10	14
		h-index	g-index

14	14	14	1293
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A Companion Guide to the String Method with Swarms of Trajectories: Characterization, Performance, and Pitfalls. Journal of Chemical Theory and Computation, 2022, 18, 1406-1422.	5.3	14
2	Accurate determination of protein:ligand standard binding free energies from molecular dynamics simulations. Nature Protocols, 2022, 17, 1114-1141.	12.0	56
3	MLCV: Bridging Machine-Learning-Based Dimensionality Reduction and Free-Energy Calculation. Journal of Chemical Information and Modeling, 2022, 62, 1-8.	5.4	23
4	Hazardous Shortcuts in Standard Binding Free Energy Calculations. Journal of Physical Chemistry Letters, 2022, 13, 6250-6258.	4.6	10
5	Accurate Estimation of Protein-ligand Binding Free Energies Based on Geometric Restraints. Acta Chimica Sinica, 2021, 79, 472.	1.4	1
6	BFEE2: Automated, Streamlined, and Accurate Absolute Binding Free-Energy Calculations. Journal of Chemical Information and Modeling, 2021, 61, 2116-2123.	5.4	35
7	Overcoming Free-Energy Barriers with a Seamless Combination of a Biasing Force and a Collective Variable-Independent Boost Potential. Journal of Chemical Theory and Computation, 2021, 17, 3886-3894.	5.3	15
8	Boosting Free-Energy Perturbation Calculations with GPU-Accelerated NAMD. Journal of Chemical Information and Modeling, 2020, 60, 5301-5307.	5.4	37
9	Finding an Optimal Pathway on a Multidimensional Free-Energy Landscape. Journal of Chemical Information and Modeling, 2020, 60, 5366-5374.	5.4	51
10	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	19.0	655
11	Tumbling of Anisole Units in Calixarene Promotes Its Shuttling in Rotaxanes. Journal of Physical Chemistry C, 2019, 123, 18050-18055.	3.1	4
12	BFEE: A User-Friendly Graphical Interface Facilitating Absolute Binding Free-Energy Calculations. Journal of Chemical Information and Modeling, 2018, 58, 556-560.	5.4	51
13	Zooming across the Free-Energy Landscape: Shaving Barriers, and Flooding Valleys. Journal of Physical Chemistry Letters, 2018, 9, 4738-4745.	4.6	100
14	ELF: An Extended-Lagrangian Free Energy Calculation Module for Multiple Molecular Dynamics Engines. Journal of Chemical Information and Modeling, 2018, 58, 1315-1318.	5.4	12