David J Hardy

List of Publications by Year
in descending order

14	3,217	933447	1199594
papers	citations	10	12
		h-index	g-index

16	16	16	3922
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	py-MCMD: Python Software for Performing Hybrid Monte Carlo/Molecular Dynamics Simulations with GOMC and NAMD. Journal of Chemical Theory and Computation, 2022, 18, 4983-4994.	5.3	10
2	AI-driven multiscale simulations illuminate mechanisms of SARS-CoV-2 spike dynamics. International Journal of High Performance Computing Applications, 2021, 35, 432-451.	3.7	91
3	Multilevel summation for periodic electrostatics using B-splines. Journal of Chemical Physics, 2021, 154, 144105.	3.0	1
4	Lessons Learned from Responsive Molecular Dynamics Studies of the COVID-19 Virus. , 2021, , .		2
5	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	3.0	1,548
6	Boosting Free-Energy Perturbation Calculations with GPU-Accelerated NAMD. Journal of Chemical Information and Modeling, 2020, 60, 5301-5307.	5.4	37
7	Multilevel summation with B-spline interpolation for pairwise interactions in molecular dynamics simulations. Journal of Chemical Physics, 2016, 144, 114112.	3.0	7
8	Multilevel Summation Method for Electrostatic Force Evaluation. Journal of Chemical Theory and Computation, 2015, 11, 766-779.	5.3	46
9	High-Performance Scalable Molecular Dynamics Simulations of a Polarizable Force Field Based on Classical Drude Oscillators in NAMD. Journal of Physical Chemistry Letters, 2011, 2, 87-92.	4.6	233
10	GPU-accelerated molecular modeling coming of age. Journal of Molecular Graphics and Modelling, 2010, 29, 116-125.	2.4	336
11	Multilevel summation of electrostatic potentials using graphics processing units. Parallel Computing, 2009, 35, 164-177.	2.1	118
12	Accelerating molecular modeling applications with graphics processors. Journal of Computational Chemistry, 2007, 28, 2618-2640.	3.3	619
13	Correcting mesh-based force calculations to conserve both energy and momentum in molecular dynamics simulations. Journal of Computational Physics, 2007, 225, 1-5.	3.8	26
14	Multiple grid methods for classical molecular dynamics. Journal of Computational Chemistry, 2002, 23, 673-684.	3.3	112