

David J Hardy

List of Publications by Year in descending order

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14
papers

3,217
citations

933447

10
h-index

1199594

12
g-index

16
all docs

16
docs citations

16
times ranked

3922
citing authors

#	ARTICLE	IF	CITATIONS
1	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	3.0	1,548
2	Accelerating molecular modeling applications with graphics processors. Journal of Computational Chemistry, 2007, 28, 2618-2640.	3.3	619
3	GPU-accelerated molecular modeling coming of age. Journal of Molecular Graphics and Modelling, 2010, 29, 116-125.	2.4	336
4	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
5	Multilevel summation of electrostatic potentials using graphics processing units. Parallel Computing, 2009, 35, 164-177.	2.1	118
6	Multiple grid methods for classical molecular dynamics. Journal of Computational Chemistry, 2002, 23, 673-684.	3.3	112
7	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
8	Multilevel Summation Method for Electrostatic Force Evaluation. Journal of Chemical Theory and Computation, 2015, 11, 766-779.	5.3	46
9	Boosting Free-Energy Perturbation Calculations with GPU-Accelerated NAMD. Journal of Chemical Information and Modeling, 2020, 60, 5301-5307.	5.4	37
10	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
11	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
12	Multilevel summation with B-spline interpolation for pairwise interactions in molecular dynamics simulations. Journal of Chemical Physics, 2016, 144, 114112.	3.0	7
13	Lessons Learned from Responsive Molecular Dynamics Studies of the COVID-19 Virus. , 2021, , .		2
14	Multilevel summation for periodic electrostatics using B-splines. Journal of Chemical Physics, 2021, 154, 144105.	3.0	1