

W Michael Brown

List of Publications by Year in descending order

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Version: 2024-02-01

21
papers

4,514
citations

623734

14
h-index

752698

20
g-index

21
all docs

21
docs citations

21
times ranked

2187
citing authors

#	ARTICLE	IF	CITATIONS
1	LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. <i>Computer Physics Communications</i> , 2022, 271, 108171.	7.5	3,106
2	Implementing molecular dynamics on hybrid high performance computers – short range forces. <i>Computer Physics Communications</i> , 2011, 182, 898-911.	7.5	549
3	Implementing molecular dynamics on hybrid high performance computers – Particle-particle particle-mesh. <i>Computer Physics Communications</i> , 2012, 183, 449-459.	7.5	373
4	Implementing molecular dynamics on hybrid high performance computers – Three-body potentials. <i>Computer Physics Communications</i> , 2013, 184, 2785-2793.	7.5	112
5	Liquid crystal nanodroplets in solution. <i>Journal of Chemical Physics</i> , 2009, 130, 044901.	3.0	73
6	New insights into the dynamics and morphology of P3HT:PCBM active layers in bulk heterojunctions. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 17873.	2.8	53
7	Optimal Neuronal Tuning for Finite Stimulus Spaces. <i>Neural Computation</i> , 2006, 18, 1511-1526.	2.2	37
8	Optimizing legacy molecular dynamics software with directive-based offload. <i>Computer Physics Communications</i> , 2015, 195, 95-101.	7.5	32
9	Designing Novel Polymers with Targeted Properties Using the Signature Molecular Descriptor. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 826-835.	5.4	31
10	Explicit Solvent Simulations of Friction between Brush Layers of Charged and Neutral Bottle-Brush Macromolecules. <i>Macromolecules</i> , 2012, 45, 8880-8891.	4.8	28
11	Accelerated application development: The ORNL Titan experience. <i>Computers and Electrical Engineering</i> , 2015, 46, 123-138.	4.8	26
12	An Evaluation of Molecular Dynamics Performance on the Hybrid Cray XK6 Supercomputer. <i>Procedia Computer Science</i> , 2012, 9, 186-195.	2.0	24
13	Rupture mechanism of liquid crystal thin films realized by large-scale molecular simulations. <i>Nanoscale</i> , 2014, 6, 3083-3096.	5.6	20
14	A Case Study of Truncated Electrostatics for Simulation of Polyelectrolyte Brushes on GPU Accelerators. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 73-83.	5.3	17
15	Prediction of $\hat{\rho}^2$ -strand packing interactions using the signature product. <i>Journal of Molecular Modeling</i> , 2006, 12, 355-361.	1.8	9
16	Creating Artificial Binding Pocket Boundaries To Improve the Efficiency of Flexible Ligand Docking. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 1412-1422.	2.8	6
17	A deterministic algorithm for constrained enumeration of transmembrane protein folds. <i>Computational Biology and Chemistry</i> , 2005, 29, 143-150.	2.3	5
18	Efficient Calculation of Molecular Properties from Simulation Using Kernel Molecular Dynamics. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 1626-1637.	5.4	5

#	ARTICLE	IF	CITATIONS
19	Disparate data fusion for protein phosphorylation prediction. Annals of Operations Research, 2010, 174, 219-235.	4.1	3
20	Increasing Molecular Dynamics Simulation Rates with an 8-Fold Increase in Electrical Power Efficiency. , 2016, , .		3
21	Genetic algorithm based task reordering to improve the performance of batch scheduled massively parallel scientific applications. Concurrency Computation Practice and Experience, 2015, 27, 4763-4783.	2.2	2