W Michael Brown

List of Publications by Year
in descending order

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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. Computer Physics Communications, 2022, 271, 108171.	7.5	3,106
2	Increasing Molecular Dynamics Simulation Rates with an 8-Fold Increase in Electrical Power Efficiency. , 2016, , .		3
3	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
4	Optimizing legacy molecular dynamics software with directive-based offload. Computer Physics Communications, 2015, 195, 95-101.	7.5	32
5	Accelerated application development: The ORNL Titan experience. Computers and Electrical Engineering, 2015, 46, 123-138.	4.8	26
6	Rupture mechanism of liquid crystal thin films realized by large-scale molecular simulations. Nanoscale, 2014, 6, 3083-3096.	5.6	20
7	A Case Study of Truncated Electrostatics for Simulation of Polyelectrolyte Brushes on GPU Accelerators. Journal of Chemical Theory and Computation, 2013, 9, 73-83.	5.3	17
8	Implementing molecular dynamics on hybrid high performance computersâ€"Three-body potentials. Computer Physics Communications, 2013, 184, 2785-2793.	7.5	112
9	New insights into the dynamics and morphology of P3HT:PCBM active layers in bulk heterojunctions. Physical Chemistry Chemical Physics, 2013, 15, 17873.	2.8	53
10	An Evaluation of Molecular Dynamics Performance on the Hybrid Cray XK6 Supercomputer. Procedia Computer Science, 2012, 9, 186-195.	2.0	24
11	Explicit Solvent Simulations of Friction between Brush Layers of Charged and Neutral Bottle-Brush Macromolecules. Macromolecules, 2012, 45, 8880-8891.	4.8	28
12	Implementing molecular dynamics on hybrid high performance computers â€“ Particleâ€“particle particle-mesh. Computer Physics Communications, 2012, 183, 449-459.	7.5	373
13	Implementing molecular dynamics on hybrid high performance computers â€“ short range forces. Computer Physics Communications, 2011, 182, 898-911.	7.5	549
14	Disparate data fusion for protein phosphorylation prediction. Annals of Operations Research, 2010, 174, 219-235.	4.1	3
15	Liquid crystal nanodroplets in solution. Journal of Chemical Physics, 2009, 130, 044901.	3.0	73
16	Efficient Calculation of Molecular Properties from Simulation Using Kernel Molecular Dynamics. Journal of Chemical Information and Modeling, 2008, 48, 1626-1637.	5.4	5
17	Designing Novel Polymers with Targeted Properties Using the Signature Molecular Descriptor. Journal of Chemical Information and Modeling, 2006, 46, 826-835.	5.4	31
18	Prediction of Î²-strand packing interactions using the signature product. Journal of Molecular Modeling, 2006, 12, 355-361.	1.8	9

#	Article	IF	Citations
19	Optimal Neuronal Tuning for Finite Stimulus Spaces. Neural Computation, 2006, 18, 1511-1526.	2.2	37
20	A deterministic algorithm for constrained enumeration of transmembrane protein folds. Computational Biology and Chemistry, 2005, 29, 143-150.	2.3	5
21	Creating Artificial Binding Pocket Boundaries To Improve the Efficiency of Flexible Ligand Docking. Journal of Chemical Information and Computer Sciences, 2004, 44, 1412-1422.	2.8	6