Christoph Junghans

List of Publications by Year
in descending order

37 papers	1,753 citations	304368 22 h-index	360668 35 g-index
40 all docs	40 docs citations	40 times ranked	1387 citing authors

#	Article	IF	Citations
1	Cabana: A Performance Portable Library for Particle-Based Simulations. Journal of Open Source Software, 2022, 7, 4115.	2.0	7
2	Enabling particle applications for exascale computing platforms. International Journal of High Performance Computing Applications, 2021, 35, 572-597.	2.4	15
3	Asynchronous distributed-memory task-parallel algorithm for compressible flows on unstructured 3D Eulerian grids. Advances in Engineering Software, 2021, 160, 102962.	1.8	7
4	Modeling and scale-bridging using machine learning: nanoconfinement effects in porous media. Scientific Reports, 2020, 10, 13312.	1.6	24
5	Multiscale simulation of plasma flows using active learning. Physical Review E, 2020, 102, 023310.	0.8	11
6	Excited-state electronic structure of molecules using many-body Greenâ€™s functions: Quasiparticles and electronâ€“hole excitations with VOTCA-XTP. Journal of Chemical Physics, 2020, 152, 114103.	1.2	20
7	ESPResSo++ 2.0: Advanced methods for multiscale molecular simulation. Computer Physics Communications, 2019, 238, 66-76.	3.0	30
8	Electronic Excitations in Complex Molecular Environments: Many-Body Greenâ€™s Functions Theory in VOTCA-XTP. Journal of Chemical Theory and Computation, 2018, 14, 6253-6268.	2.3	28
9	Adaptive resolution molecular dynamics technique: Down to the essential. Journal of Chemical Physics, 2018, 149, 024104.	1.2	30
10	Computational efficiency and Amdahlâ€™s law for the adaptive resolution simulation technique. Computer Physics Communications, 2017, 215, 20-25.	3.0	5
11	Scalable and fast heterogeneous molecular simulation with predictive parallelization schemes. Physical Review E, 2017, 96, 053311.	0.8	9
12	Accommodating Thread-Level Heterogeneity in Coupled Parallel Applications. , 2017, , .		4
13	C â€“IBI: Targeting cumulative coordination within an iterative protocol to derive coarse-grained models of (multi-component) complex fluids. Journal of Chemical Physics, 2016, 144, 174106.	1.2	24
14	Database assisted distribution to improve fault tolerance for multiphysics applications. , 2015, , .		6
15	TADSim. ACM Transactions on Modeling and Computer Simulation, 2015, 25, 1-26.	0.6	12
16	Distributed Database Kriging for Adaptive Sampling (D2KAS). Computer Physics Communications, 2015, 192, 138-147.	3.0	23
17	STOCK: Structure mapper and online coarse-graining kit for molecular simulations. Journal of Computational Chemistry, 2015, 36, 467-477.	1.5	11
18	Relative Entropy and Optimization-Driven Coarse-Graining Methods in VOTCA. PLoS ONE, 2015, 10, e0131754.	1.1	55

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19	Molecular Dynamics in the Multicanonical Ensemble: Equivalence of Wangâ€“Landau Sampling, Statistical Temperature Molecular Dynamics, and Metadynamics. Journal of Chemical Theory and Computation, 2014, 10, 1843-1847.	2.3	38
20	Spatial adaptive sampling in multiscale simulation. Computer Physics Communications, 2014, 185, 1857-1864.	3.0	23
21	Multiscale Simulation of Liquid Water Using a Four-to-One Mapping for Coarse-Graining. Journal of Chemical Theory and Computation, 2013, 9, 5168-5175.	2.3	19
22	Adaptive resolution simulation of salt solutions. New Journal of Physics, 2013, 15, 105007.	1.2	24
23	Adaptive resolution molecular dynamics simulation through coupling to an internal particle reservoir. Physical Review Letters, 2012, 108, 170602.	2.9	126
24	Structure Formation of Toluene around C60: Implementation of the Adaptive Resolution Scheme (AdResS) into GROMACS. Journal of Chemical Theory and Computation, 2012, 8, 398-403.	2.3	52
25	Kirkwoodâ€“Buff Coarse-Grained Force Fields for Aqueous Solutions. Journal of Chemical Theory and Computation, 2012, 8, 1802-1807.	2.3	62
26	Hybrid Approaches to Coarseâ€Graining using the VOTCA Package: Liquid Hexane. Macromolecular Theory and Simulations, 2011, 20, 472-477.	0.6	44
27	Hierarchies in nucleation transitions. Computer Physics Communications, 2011, 182, 1937-1940.	3.0	12
28	A reference implementation of the adaptive resolution scheme in ESPResSo. Computer Physics Communications, 2010, 181, 1449-1454.	3.0	19
29	Communication: On the locality of Hydrogen bond networks at hydrophobic interfaces. Journal of Chemical Physics, 2010, 133, 221101.	1.2	55
30	Comparative atomistic and coarse-grained study of water: What do we lose by coarse-graining?. European Physical Journal E, 2009, 28, 221-229.	0.7	231
31	Versatile Object-Oriented Toolkit for Coarse-Graining Applications. Journal of Chemical Theory and Computation, 2009, 5, 3211-3223.	2.3	390
32	Statistical mechanics of aggregation and crystallization for semiflexible polymers. Europhysics Letters, 2009, 87, 40002.	0.7	38
33	Simulation approaches to soft matter: Generic statistical properties vs. chemical details. Computer Physics Communications, 2008, 179, 51-60.	3.0	24
34	Thermodynamics of peptide aggregation processes: An analysis from perspectives of three statistical ensembles. Journal of Chemical Physics, 2008, 128, 085103.	1.2	50
35	Transport properties controlled by a thermostat: An extended dissipative particle dynamics thermostat. Soft Matter, 2008, 4, 156-161.	1.2	113
36	Microcanonical Analyses of Peptide Aggregation Processes. Physical Review Letters, 2006, 97, 218103.	2.9	101

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37	NUMERICAL COMPARISON OF WANGâ€“LANDAU SAMPLING AND PARALLEL TEMPERING FOR MET-ENKEPHALIN. International Journal of Modern Physics C, 2006, 17, 817-824.	0.8	11