Christoph Junghans

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7624219/publications.pdf

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37	1,753	304602 22	360920 35
papers	citations	h-index	g-index

40	40	40	1387
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Versatile Object-Oriented Toolkit for Coarse-Graining Applications. Journal of Chemical Theory and Computation, 2009, 5, 3211-3223.	2.3	390
2	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
3	Adaptive resolution molecular dynamics simulation through coupling to an internal particle reservoir. Physical Review Letters, 2012, 108, 170602.	2.9	126
4	Transport properties controlled by a thermostat: An extended dissipative particle dynamics thermostat. Soft Matter, 2008, 4, 156-161.	1.2	113
5	Microcanonical Analyses of Peptide Aggregation Processes. Physical Review Letters, 2006, 97, 218103.	2.9	101
6	Kirkwoodâ€“Buff Coarse-Grained Force Fields for Aqueous Solutions. Journal of Chemical Theory and Computation, 2012, 8, 1802-1807.	2.3	62
7	Communication: On the locality of Hydrogen bond networks at hydrophobic interfaces. Journal of Chemical Physics, 2010, 133, 221101.	1.2	55
8	Relative Entropy and Optimization-Driven Coarse-Graining Methods in VOTCA. PLoS ONE, 2015, 10, e0131754.	1.1	55
9	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
10	Thermodynamics of peptide aggregation processes: An analysis from perspectives of three statistical ensembles. Journal of Chemical Physics, 2008, 128, 085103.	1.2	50
11	Hybrid Approaches to Coarseâ€Graining using the VOTCA Package: Liquid Hexane. Macromolecular Theory and Simulations, 2011, 20, 472-477.	0.6	44
12	Statistical mechanics of aggregation and crystallization for semiflexible polymers. Europhysics Letters, 2009, 87, 40002.	0.7	38
13	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
14	Adaptive resolution molecular dynamics technique: Down to the essential. Journal of Chemical Physics, 2018, 149, 024104.	1.2	30
15	ESPResSo++ 2.0: Advanced methods for multiscale molecular simulation. Computer Physics Communications, 2019, 238, 66-76.	3.0	30
16	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
17	Simulation approaches to soft matter: Generic statistical properties vs. chemical details. Computer Physics Communications, 2008, 179, 51-60.	3.0	24
18	Adaptive resolution simulation of salt solutions. New Journal of Physics, 2013, 15, 105007.	1.2	24

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19	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
20	Modeling and scale-bridging using machine learning: nanoconfinement effects in porous media. Scientific Reports, 2020, 10, 13312.	1.6	24
21	Spatial adaptive sampling in multiscale simulation. Computer Physics Communications, 2014, 185, 1857-1864.	3.0	23
22	Distributed Database Kriging for Adaptive Sampling (D2KAS). Computer Physics Communications, 2015, 192, 138-147.	3.0	23
23	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
24	A reference implementation of the adaptive resolution scheme in ESPResSo. Computer Physics Communications, 2010, 181, 1449-1454.	3.0	19
25	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
26	Enabling particle applications for exascale computing platforms. International Journal of High Performance Computing Applications, 2021, 35, 572-597.	2.4	15
27	Hierarchies in nucleation transitions. Computer Physics Communications, 2011, 182, 1937-1940.	3.0	12
28	TADSim. ACM Transactions on Modeling and Computer Simulation, 2015, 25, 1-26.	0.6	12
29	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
30	STOCK: Structure mapper and online coarse-graining kit for molecular simulations. Journal of Computational Chemistry, 2015, 36, 467-477.	1.5	11
31	Multiscale simulation of plasma flows using active learning. Physical Review E, 2020, 102, 023310.	0.8	11
32	Scalable and fast heterogeneous molecular simulation with predictive parallelization schemes. Physical Review E, 2017, 96, 053311.	0.8	9
33	Asynchronous distributed-memory task-parallel algorithm for compressible flows on unstructured 3D Eulerian grids. Advances in Engineering Software, 2021, 160, 102962.	1.8	7
34	Cabana: A Performance Portable Library for Particle-Based Simulations. Journal of Open Source Software, 2022, 7, 4115.	2.0	7
35	Database assisted distribution to improve fault tolerance for multiphysics applications. , 2015, , .		6
36	Computational efficiency and Amdahlâ€™s law for the adaptive resolution simulation technique. Computer Physics Communications, 2017, 215, 20-25.	3.0	5

#	Article	IF	Citations
37	Accommodating Thread-Level Heterogeneity in Coupled Parallel Applications. , 2017, , .		4