Matej Praprotnik

List of Publications by Year in descending order

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75 papers	2,946 citations	172457 29 h-index	161849 54 g-index
75 all docs	75 docs citations	75 times ranked	1772 citing authors

#	Article	IF	Citations
1	Multiscale Simulation of Soft Matter: From Scale Bridging to Adaptive Resolution. Annual Review of Physical Chemistry, 2008, 59, 545-571.	10.8	410
2	Adaptive resolution molecular-dynamics simulation: Changing the degrees of freedom on the fly. Journal of Chemical Physics, 2005, 123, 224106.	3.0	347
3	Temperature Dependence of Water Vibrational Spectrum:Â A Molecular Dynamics Simulation Study. Journal of Physical Chemistry A, 2004, 108, 11056-11062.	2.5	147
4	Transport properties controlled by a thermostat: An extended dissipative particle dynamics thermostat. Soft Matter, 2008, 4, 156-161.	2.7	113
5	Adaptive resolution scheme for efficient hybrid atomistic-mesoscale molecular dynamics simulations of dense liquids. Physical Review E, 2006, 73, 066701.	2.1	110
6	Concurrent triple-scale simulation of molecular liquids. Journal of Chemical Physics, 2008, 128, 114110.	3.0	104
7	Coupling different levels of resolution in molecular simulations. Journal of Chemical Physics, 2010, 132, 114101.	3.0	93
8	Adaptive resolution simulation of liquid water. Journal of Physics Condensed Matter, 2007, 19, 292201.	1.8	85
9	Molecular dynamics integration and molecular vibrational theory. III. The infrared spectrum of water. Journal of Chemical Physics, 2005, 122, 174103.	3.0	81
10	A macromolecule in a solvent: Adaptive resolution molecular dynamics simulation. Journal of Chemical Physics, 2007, 126, 134902.	3.0	78
11	Adaptive resolution simulation of an atomistic protein in MARTINI water. Journal of Chemical Physics, 2014, 140, 054114.	3.0	74
12	Coupling atomistic and continuum hydrodynamics through a mesoscopic model: Application to liquid water. Journal of Chemical Physics, 2009, 131, 244107.	3.0	73
13	Modeling diffusive dynamics in adaptive resolution simulation of liquid water. Journal of Chemical Physics, 2008, 128, 024503.	3.0	66
14	Molecular systems with open boundaries: Theory and simulation. Physics Reports, 2017, 693, 1-56.	25.6	66
15	ENZO: A Web Tool for Derivation and Evaluation of Kinetic Models of Enzyme Catalyzed Reactions. PLoS ONE, 2011, 6, e22265.	2.5	65
16	Molecular dynamics integration and molecular vibrational theory. I. New symplectic integrators. Journal of Chemical Physics, 2005, 122, 174101.	3.0	54
17	Adaptive molecular resolution via a continuous change of the phase space dimensionality. Physical Review E, 2007, 75, 017701.	2.1	49
18	Adaptive Resolution Simulation of MARTINI Solvents. Journal of Chemical Theory and Computation, 2014, 10, 2591-2598.	5.3	46

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19	Adaptive Resolution Simulation of a DNA Molecule in Salt Solution. Journal of Chemical Theory and Computation, 2015, 11, 5035-5044.	5.3	46
20	Open boundary molecular dynamics. European Physical Journal: Special Topics, 2015, 224, 2331-2349.	2.6	44
21	Fractional dimensions of phase space variables: a tool for varying the degrees of freedom of a system in a multiscale treatment. Journal of Physics A: Mathematical and Theoretical, 2007, 40, F281-F288.	2.1	40
22	Adaptive resolution simulation of polarizable supramolecular coarse-grained water models. Journal of Chemical Physics, 2015, 142, 244118.	3.0	39
23	Open boundary molecular dynamics of sheared star-polymer melts. Soft Matter, 2016, 12, 2416-2439.	2.7	39
24	Multiscale simulation of water flow past a C540 fullerene. Journal of Computational Physics, 2012, 231, 2677-2681.	3.8	37
25	Molecular dynamics integration and molecular vibrational theory. II. Simulation of nonlinear molecules. Journal of Chemical Physics, 2005, 122, 174102.	3.0	35
26	Statistical Physics Problems in Adaptive Resolution Computer Simulations of Complex Fluids. Journal of Statistical Physics, 2011, 145, 946-966.	1.2	34
27	Adaptive Resolution Simulation of Supramolecular Water: The Concurrent Making, Breaking, and Remaking of Water Bundles. Journal of Chemical Theory and Computation, 2016, 12, 4138-4145.	5.3	30
28	Deciphering the dynamics of star molecules in shear flow. Soft Matter, 2017, 13, 4971-4987.	2.7	30
29	Adaptive resolution molecular dynamics technique: Down to the essential. Journal of Chemical Physics, 2018, 149, 024104.	3.0	30
30	Comment on â€œAdaptive Multiscale Molecular Dynamics of Macromolecular Fluidsâ€• Physical Review Letters, 2011, 107, 099801; discussion 099802.	7.8	29
31	Order and interactions in DNA arrays: Multiscale molecular dynamics simulation. Scientific Reports, 2017, 7, 4775.	3.3	27
32	Adaptive resolution simulation of an atomistic DNA molecule in MARTINI salt solution. European Physical Journal: Special Topics, 2016, 225, 1595-1607.	2.6	25
33	Simulation approaches to soft matter: Generic statistical properties vs. chemical details. Computer Physics Communications, 2008, 179, 51-60.	7.5	24
34	Adaptive resolution simulation of salt solutions. New Journal of Physics, 2013, 15, 105007.	2.9	24
35	Continuum simulations of water flow in carbon nanotube membranes. New Journal of Physics, 2014, 16, 082001.	2.9	23
36	Adaptive resolution simulations coupling atomistic water to dissipative particle dynamics. Journal of Chemical Physics, 2017, 147, 114110.	3.0	22

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37	Open-Boundary Molecular Dynamics of a DNA Molecule in a Hybrid Explicit/Implicit Salt Solution. Biophysical Journal, 2018, 114, 2352-2362.	0.5	22
38	Application of the Eckart frame to soft matter: rotation of star polymers under shear flow. Soft Matter, 2017, 13, 6988-7000.	2.7	21
39	Adaptive resolution simulations of biomolecular systems. European Biophysics Journal, 2017, 46, 821-835.	2.2	20
40	On phonons and water flow enhancement in carbon nanotubes. Nature Nanotechnology, 2017, 12, 1106-1108.	31.5	19
41	Multiscale Simulation of Protein Hydration Using the SWINGER Dynamical Clustering Algorithm. Journal of Chemical Theory and Computation, 2018, 14, 1754-1761.	5.3	19
42	Molecular Dynamics Integration Meets Standard Theory of Molecular Vibrations. Journal of Chemical Information and Modeling, 2005, 45, 1571-1579.	5.4	17
43	Accelerated Simulations of Molecular Systems through Learning of Effective Dynamics. Journal of Chemical Theory and Computation, 2022, 18, 538-549.	5.3	17
44	From adaptive resolution to molecular dynamics of open systems. European Physical Journal B, 2021, 94, 189.	1.5	14
45	Symplectic molecular dynamics integration using normal mode analysis. International Journal of Quantum Chemistry, 2001, 84, 2-12.	2.0	12
46	Molecular Dynamics Integration Time Step Dependence of the Split Integration Symplectic Method on System Density. Journal of Chemical Information and Computer Sciences, 2003, 43, 1922-1927.	2.8	12
47	Molecular Dynamics Simulation of High Density DNA Arrays. Computation, 2018, 6, 3.	2.0	12
48	Particleâ€“Continuum Coupling and its Scaling Regimes: Theory and Applications. Advanced Theory and Simulations, 2020, 3, 1900232.	2.8	12
49	Implementation and evaluation of MPI-based parallel MD program. International Journal of Quantum Chemistry, 2001, 84, 23-31.	2.0	11
50	New all-atom force field for molecular dynamics simulation of an AlPO4-34 molecular sieve. Journal of Computational Chemistry, 2008, 29, 122-129.	3.3	11
51	STOCK: Structure mapper and online coarse-graining kit for molecular simulations. Journal of Computational Chemistry, 2015, 36, 467-477.	3.3	11
52	SWINGER: a clustering algorithm for concurrent coupling of atomistic and supramolecular liquids. Interface Focus, 2019, 9, 20180075.	3.0	11
53	Tuning the Dielectric Response of Water in Nanoconfinement through Surface Wettability. ACS Nano, 2021, 15, 20311-20318.	14.6	10
54	Continuum simulations of water flow past fullerene molecules. European Physical Journal: Special Topics, 2015, 224, 2321-2330.	2.6	8

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55	Splayâ€“density coupling in semiflexible main-chain nematic polymers with hairpins. Soft Matter, 2018, 14, 5898-5905.	2.7	8
56	Multiscale Molecular Modeling. Methods in Molecular Biology, 2013, 924, 567-583.	0.9	7
57	Back-mapping augmented adaptive resolution simulation. Journal of Chemical Physics, 2020, 153, 164118.	3.0	7
58	Parallel programming library for molecular dynamics simulations. International Journal of Quantum Chemistry, 2004, 96, 530-536.	2.0	6
59	Adaptive Resolution Molecular Dynamics Technique. , 2018, , 1-15.		3
60	Lessons learned from urgent computing in Europe: Tackling the COVID-19 pandemic. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	3
61	Dissipative Particle Dynamics Simulation of Ultrasound Propagation through Liquid Water. Journal of Chemical Theory and Computation, 2022, 18, 1227-1240.	5.3	3
62	Adaptive resolution simulation of liquid water. Journal of Physics Condensed Matter, 2008, 21, 499801-499801.	1.8	2
63	Reply to comments by R. Klein on â€œOpen boundary molecular dynamicsâ€• European Physical Journal: Special Topics, 2015, 224, 2511-2513.	2.6	2
64	Densityâ€“Nematic Coupling in Isotropic Linear Polymers: Acoustic and Osmotic Birefringence. Advanced Theory and Simulations, 2019, 2, 1900019.	2.8	2
65	Domain Decomposition Methods for Multiscale Modeling. , 2020, , 2551-2571.		2
66	Adaptive Resolution Molecular Dynamics Technique. , 2020, , 1443-1457.		1
67	The split integration symplectic method. Cellular and Molecular Biology Letters, 2002, 7, 147-8.	7.0	1
68	Suspension of discrete microscopic oscillators as a model of an ultrasonic metafluid. Physical Review B, 2022, 105, .	3.2	1
69	Contributory presentations/posters. Journal of Biosciences, 1999, 24, 33-198.	1.1	0
70	Molecular Modelingâ€”A New Approach. AIP Conference Proceedings, 2007, , .	0.4	0
71	Parallel Approaches in Molecular Dynamics Simulations. , 2009, , 281-305.		0
72	Recent algorithmic development of parallel force decomposition and Hamiltonian splitting methods for macromolecular simulation. , 2012, , .		0

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73	Extending the Adress Multiscale Scheme for Protein and Bilayer Applications. Biophysical Journal, 2016, 110, 643a-644a.	0.5	0
74	Domain Decomposition Methods for Multiscale Modeling. , 2018, , 1-21.		0
75	Isotropic Polymers: Densityâ€“Nematic Coupling in Isotropic Linear Polymers: Acoustic and Osmotic Birefringence (Adv. Theory Simul. 5/2019). Advanced Theory and Simulations, 2019, 2, 1970016.	2.8	0