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	Dissipative Particle Dynamics Simulation of Ultrasound Propagation through Liquid Water. Journal of Chemical Theory and Computation, 2022, 18, 1227-1240.	5.3	3
2	Accelerated Simulations of Molecular Systems through Learning of Effective Dynamics. Journal of Chemical Theory and Computation, 2022, 18, 538-549.	5.3	17
3	Suspension of discrete microscopic oscillators as a model of an ultrasonic metafluid. Physical Review B, 2022, 105, .	3.2	1
4	From adaptive resolution to molecular dynamics of open systems. European Physical Journal B, 2021, 94, 189.	1.5	14
5	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
6	Tuning the Dielectric Response of Water in Nanoconfinement through Surface Wettability. ACS Nano, 2021, 15, 20311-20318.	14.6	10
7	Back-mapping augmented adaptive resolution simulation. Journal of Chemical Physics, 2020, 153, 164118.	3.0	7
8	Particleâ€“Continuum Coupling and its Scaling Regimes: Theory and Applications. Advanced Theory and Simulations, 2020, 3, 1900232.	2.8	12
9	Domain Decomposition Methods for Multiscale Modeling. , 2020, , 2551-2571.		2
10	Adaptive Resolution Molecular Dynamics Technique. , 2020, , 1443-1457.		1
11	Densityâ€“Nematic Coupling in Isotropic Linear Polymers: Acoustic and Osmotic Birefringence. Advanced Theory and Simulations, 2019, 2, 1900019.	2.8	2
12	SWINGER: a clustering algorithm for concurrent coupling of atomistic and supramolecular liquids. Interface Focus, 2019, 9, 20180075.	3.0	11
13	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
14	Multiscale Simulation of Protein Hydration Using the SWINGER Dynamical Clustering Algorithm. Journal of Chemical Theory and Computation, 2018, 14, 1754-1761.	5.3	19
15	Open-Boundary Molecular Dynamics of a DNA Molecule in a Hybrid Explicit/Implicit Salt Solution. Biophysical Journal, 2018, 114, 2352-2362.	0.5	22
16	Adaptive Resolution Molecular Dynamics Technique. , 2018, , 1-15.		3
17	Splayâ€“density coupling in semiflexible main-chain nematic polymers with hairpins. Soft Matter, 2018, 14, 5898-5905.	2.7	8
18	Molecular Dynamics Simulation of High Density DNA Arrays. Computation, 2018, 6, 3.	2.0	12

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19	Domain Decomposition Methods for Multiscale Modeling. , 2018, , 1-21.		0
20	Adaptive resolution molecular dynamics technique: Down to the essential. Journal of Chemical Physics, 2018, 149, 024104.	3.0	30
21	Deciphering the dynamics of star molecules in shear flow. Soft Matter, 2017, 13, 4971-4987.	2.7	30
22	Adaptive resolution simulations coupling atomistic water to dissipative particle dynamics. Journal of Chemical Physics, 2017, 147, 114110.	3.0	22
23	Adaptive resolution simulations of biomolecular systems. European Biophysics Journal, 2017, 46, 821-835.	2.2	20
24	Application of the Eckart frame to soft matter: rotation of star polymers under shear flow. Soft Matter, 2017, 13, 6988-7000.	2.7	21
25	Order and interactions in DNA arrays: Multiscale molecular dynamics simulation. Scientific Reports, 2017, 7, 4775.	3.3	27
26	On phonons and water flow enhancement in carbon nanotubes. Nature Nanotechnology, 2017, 12, 1106-1108.	31.5	19
27	Molecular systems with open boundaries: Theory and simulation. Physics Reports, 2017, 693, 1-56.	25.6	66
28	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
29	Adaptive resolution simulation of an atomistic DNA molecule in MARTINI salt solution. European Physical Journal: Special Topics, 2016, 225, 1595-1607.	2.6	25
30	Extending the Adress Multiscale Scheme for Protein and Bilayer Applications. Biophysical Journal, 2016, 110, 643a-644a.	0.5	0
31	Open boundary molecular dynamics of sheared star-polymer melts. Soft Matter, 2016, 12, 2416-2439.	2.7	39
32	Reply to comments by R. Klein on â€œOpen boundary molecular dynamicsâ€• European Physical Journal: Special Topics, 2015, 224, 2511-2513.	2.6	2
33	Open boundary molecular dynamics. European Physical Journal: Special Topics, 2015, 224, 2331-2349.	2.6	44
34	Adaptive resolution simulation of polarizable supramolecular coarse-grained water models. Journal of Chemical Physics, 2015, 142, 244118.	3.0	39
35	Adaptive Resolution Simulation of a DNA Molecule in Salt Solution. Journal of Chemical Theory and Computation, 2015, 11, 5035-5044.	5.3	46
36	Continuum simulations of water flow past fullerene molecules. European Physical Journal: Special Topics, 2015, 224, 2321-2330.	2.6	8

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37	STOCK: Structure mapper and online coarse-graining kit for molecular simulations. Journal of Computational Chemistry, 2015, 36, 467-477.	3.3	11
38	Continuum simulations of water flow in carbon nanotube membranes. New Journal of Physics, 2014, 16, 082001.	2.9	23
39	Adaptive resolution simulation of an atomistic protein in MARTINI water. Journal of Chemical Physics, 2014, 140, 054114.	3.0	74
40	Adaptive Resolution Simulation of MARTINI Solvents. Journal of Chemical Theory and Computation, 2014, 10, 2591-2598.	5.3	46
41	Multiscale Molecular Modeling. Methods in Molecular Biology, 2013, 924, 567-583.	0.9	7
42	Adaptive resolution simulation of salt solutions. New Journal of Physics, 2013, 15, 105007.	2.9	24
43	Recent algorithmic development of parallel force decomposition and Hamiltonian splitting methods for macromolecular simulation. , 2012, , .		0
44	Multiscale simulation of water flow past a C540 fullerene. Journal of Computational Physics, 2012, 231, 2677-2681.	3.8	37
45	ENZO: A Web Tool for Derivation and Evaluation of Kinetic Models of Enzyme Catalyzed Reactions. PLoS ONE, 2011, 6, e22265.	2.5	65
46	Statistical Physics Problems in Adaptive Resolution Computer Simulations of Complex Fluids. Journal of Statistical Physics, 2011, 145, 946-966.	1.2	34
47	Comment on â€œAdaptive Multiscale Molecular Dynamics of Macromolecular Fluidsâ€• Physical Review Letters, 2011, 107, 099801; discussion 099802.	7.8	29
48	Coupling different levels of resolution in molecular simulations. Journal of Chemical Physics, 2010, 132, 114101.	3.0	93
49	Parallel Approaches in Molecular Dynamics Simulations. , 2009, , 281-305.		0
50	Coupling atomistic and continuum hydrodynamics through a mesoscopic model: Application to liquid water. Journal of Chemical Physics, 2009, 131, 244107.	3.0	73
51	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
52	Simulation approaches to soft matter: Generic statistical properties vs. chemical details. Computer Physics Communications, 2008, 179, 51-60.	7.5	24
53	Multiscale Simulation of Soft Matter: From Scale Bridging to Adaptive Resolution. Annual Review of Physical Chemistry, 2008, 59, 545-571.	10.8	410
54	Transport properties controlled by a thermostat: An extended dissipative particle dynamics thermostat. Soft Matter, 2008, 4, 156-161.	2.7	113

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55	Concurrent triple-scale simulation of molecular liquids. Journal of Chemical Physics, 2008, 128, 114110.	3.0	104
56	Modeling diffusive dynamics in adaptive resolution simulation of liquid water. Journal of Chemical Physics, 2008, 128, 024503.	3.0	66
57	Adaptive resolution simulation of liquid water. Journal of Physics Condensed Matter, 2008, 21, 499801-499801.	1.8	2
58	Adaptive resolution simulation of liquid water. Journal of Physics Condensed Matter, 2007, 19, 292201.	1.8	85
59	Adaptive molecular resolution via a continuous change of the phase space dimensionality. Physical Review E, 2007, 75, 017701.	2.1	49
60	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
61	A macromolecule in a solvent: Adaptive resolution molecular dynamics simulation. Journal of Chemical Physics, 2007, 126, 134902.	3.0	78
62	Molecular Modelingâ€"A New Approach. AIP Conference Proceedings, 2007, , .	0.4	0
63	Adaptive resolution scheme for efficient hybrid atomistic-mesoscale molecular dynamics simulations of dense liquids. Physical Review E, 2006, 73, 066701.	2.1	110
64	Adaptive resolution molecular-dynamics simulation: Changing the degrees of freedom on the fly. Journal of Chemical Physics, 2005, 123, 224106.	3.0	347
65	Molecular dynamics integration and molecular vibrational theory. II. Simulation of nonlinear molecules. Journal of Chemical Physics, 2005, 122, 174102.	3.0	35
66	Molecular dynamics integration and molecular vibrational theory. III. The infrared spectrum of water. Journal of Chemical Physics, 2005, 122, 174103.	3.0	81
67	Molecular dynamics integration and molecular vibrational theory. I. New symplectic integrators. Journal of Chemical Physics, 2005, 122, 174101.	3.0	54
68	Molecular Dynamics Integration Meets Standard Theory of Molecular Vibrations. Journal of Chemical Information and Modeling, 2005, 45, 1571-1579.	5.4	17
69	Parallel programming library for molecular dynamics simulations. International Journal of Quantum Chemistry, 2004, 96, 530-536.	2.0	6
70	Temperature Dependence of Water Vibrational Spectrum:Â A Molecular Dynamics Simulation Study. Journal of Physical Chemistry A, 2004, 108, 11056-11062.	2.5	147
71	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
72	The split integration symplectic method. Cellular and Molecular Biology Letters, 2002, 7, 147-8.	7.0	1

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73	Symplectic molecular dynamics integration using normal mode analysis. International Journal of Quantum Chemistry, 2001, 84, 2-12.	2.0	12
74	Implementation and evaluation of MPI-based parallel MD program. International Journal of Quantum Chemistry, 2001, 84, 23-31.	2.0	11
75	Contributory presentations/posters. Journal of Biosciences, 1999, 24, 33-198.	1.1	0