ESPResSo 4.0 â€“ an extensible software package for sim

European Physical Journal: Special Topics
227, 1789-1816
DOI: 10.1140/epjst/e2019-800186-9

Citation Report

#	Article	IF	Citations
1	A computational model for bacterial run-and-tumble motion. Journal of Chemical Physics, 2019, 150, 174111.	1.2	12
2	Modeling Gel Swelling Equilibrium in the Mean Field: From Explicit to Poisson-Boltzmann Models. Physical Review Letters, 2019, 122, 208002.	2.9	14
3	Molecular Dynamics Simulations of Ionic Liquids and Electrolytes Using Polarizable Force Fields. Chemical Reviews, 2019, 119, 7940-7995.	23.0	386
4	Particle methods in natural science and engineering. European Physical Journal: Special Topics, 2019, 227, 1493-1499.	1.2	2
5	Cell Model Approaches for Predicting the Swelling and Mechanical Properties of Polyelectrolyte Gels. Macromolecules, 2019, 52, 9341-9353.	2.2	9
6	Suspensions of magnetic nanogels at zero field: Equilibrium structural properties. Journal of Magnetism and Magnetic Materials, 2020, 498, 166152.	1.0	6
7	Interparticle correlations in the simple cubic lattice of ferroparticles: Theory and computer simulations. Physica A: Statistical Mechanics and Its Applications, 2020, 558, 124923.	1.2	8
8	How to speed up ion transport in nanopores. Nature Communications, 2020, 11, 6085.	5.8	57
9	Coarse-Grained Modeling of Pore Dynamics on the Red Blood Cell Membrane under Large Deformations. Biophysical Journal, 2020, 119, 471-482.	0.2	20
10	Nanoparticle-assisted polymer translocation through a nanopore. Polymer, 2020, 204, 122847.	1.8	4
11	Directing the Diffusion of a Nonmagnetic Nanosized Active Particle with External Magnetic Fields. Journal of Physical Chemistry B, 2020, 124, 8188-8197.	1.2	4
12	Stabilizing Leaflet Asymmetry under Differential Stress in a Highly Coarse-Grained Lipid Membrane Model. Journal of Chemical Theory and Computation, 2020, 16, 7195-7206.	2.3	11
13	Pore shapes effects on polymer translocation. European Physical Journal E, 2020, 43, 76.	0.7	1
14	Interface Counterion Localization Induces a Switch between Tight and Loose Configurations of Knotted Weak Polyacid Rings despite Intermonomer Coulomb Repulsions. Journal of Physical Chemistry B, 2020, 124, 2930-2937.	1.2	5
15	Chromosome Segregation in Bacillus subtilis Follows an Overall Pattern of Linear Movement and Is Highly Robust against Cell Cycle Perturbations. MSphere, 2020, 5, .	1.3	13
16	Diffusion of single active-dipolar cubes in applied fields. Journal of Molecular Liquids, 2020, 304, 112688.	2.3	5
17	Studying rare events using forward-flux sampling: Recent breakthroughs and future outlook. Journal of Chemical Physics, 2020, 152, 060901.	1.2	50
18	Understanding and Controlling Food Protein Structure and Function in Foods: Perspectives from Experiments and Computer Simulations. Annual Review of Food Science and Technology, 2020, 11, 365-387.	5.1	33

#	Article	IF	Citations
19	Springâ€network model of red blood cell: From membrane mechanics to validation. International Journal for Numerical Methods in Fluids, 2020, 92, 1368-1393.	0.9	14
20	Computational Modeling of Blood Flow with Rare Cell in a Microbifurcation. Lecture Notes in Computational Vision and Biomechanics, 2020, , 518-525.	0.5	1
21	The influence of an applied magnetic field on the self-assembly of magnetic nanogels. Journal of Molecular Liquids, 2020, 307, 112902.	2.3	16
22	CAVIAR: A simulation package for charged particles in environments surrounded by conductive boundaries. AIP Advances, 2020, 10, 035310.	0.6	4
23	Grand-Reaction Method for Simulations of Ionization Equilibria Coupled to Ion Partitioning. Macromolecules, 2020, 53, 3007-3020.	2.2	44
24	Capture of rod-like molecules by a nanopore: Defining an â€œorientational capture radiusâ€. Journal of Chemical Physics, 2020, 152, 144902.	1.2	16
25	Computer modeling of polymer stars in variable solvent conditions: a comparison of MD simulations, self-consistent field (SCF) modeling and novel hybrid Monte Carlo SCF approach. Soft Matter, 2021, 17, 580-591.	1.2	3
26	Can oppositely charged polyelectrolyte stars form a gel? A simulational study. Soft Matter, 2021, 17, 1574-1588.	1.2	6
27	The Presence of a Wall Enhances the Probability for Ringâ€Closing Metathesis: Insights from Classical Polymer Theory and Atomistic Simulations. Macromolecular Theory and Simulations, 2021, 30, 2000076.	0.6	1
28	Quantitative prediction of charge regulation in oligopeptides. Molecular Systems Design and Engineering, 2021, 6, 122-131.	1.7	18
29	Frequency-dependent magnetic susceptibility of magnetic nanoparticles in a polymer solution: a simulation study. Soft Matter, 2021, 17, 174-183.	1.2	17
30	pH-Dependent Structure of Block Copolymer Micelles Featuring a Polyampholyte Corona: A Combined Experimental and Theoretical Approach. Macromolecules, 2021, 54, 1976-1991.	2.2	2
31	Rayleighâ€“Plateau instability of anisotropic interfaces. Part 1. An analytical and numerical study of fluid interfaces. Journal of Fluid Mechanics, 2021, 910, .	1.4	10
32	Flux and separation of magneto-active superballs in applied fields. Physical Chemistry Chemical Physics, 2021, 23, 23827-23835.	1.3	3
33	Reversible heat production during electric double layer buildup depends sensitively on the electrolyte and its reservoir. Journal of Chemical Physics, 2021, 154, 064901.	1.2	6
34	Modeling the current modulation of bundled DNA structures in nanopores. Journal of Chemical Physics, 2021, 154, 054901.	1.2	4
35	Molecular dynamics model for the antibactericity of textured surfaces. Colloids and Surfaces B: Biointerfaces, 2021, 199, 111504.	2.5	8
36	AutoPas in ls1 mardyn: Massively parallel particle simulations with node-level auto-tuning. Journal of Computational Science, 2021, 50, 101296.	1.5	6

#	Article	IF	Citations
37	Bayesian unsupervised learning reveals hidden structure in concentrated electrolytes. Journal of Chemical Physics, 2021, 154, 134902.	1.2	9
38	Molecular Simulation of Electrode-Solution Interfaces. Annual Review of Physical Chemistry, 2021, 72, 189-212.	4.8	64
39	Electrostatically Cross-Linked Reversible Gelsâ€"Effects of pH and Ionic Strength. Macromolecules, 2021, 54, 4769-4781.	2.2	15
40	Field-theoretic simulations beyond Î´-interactions: Overcoming the inverse potential problem in auxiliary field models. Journal of Chemical Physics, 2021, 155, 024106.	1.2	7
41	The nanofluids application in a twin-screw electromechanical hydrolyser. , 2021, , .		1
42	Magnetic field controlled behavior of magnetic gels studied using particle-based simulations. ChemistrySelect, 2023, 8, 1465-1486.	0.7	2
43	Numerical simulation of intracellular drug delivery via rapid squeezing. Biomicrofluidics, 2021, 15, 044102.	1.2	6
44	Leesâ€"Edwards boundary conditions for translation invariant shear flow: Implementation and transport properties. Physics of Fluids, 2021, 33, .	1.6	4
45	Field-induced response of non-spherical magnetopolymersomes: Coarse-grained molecular dynamics model. AIP Conference Proceedings, 2021, , .	0.3	0
46	Role of pKA in Charge Regulation and Conformation of Various Peptide Sequences. Polymers, 2021, 13, 214.	2.0	24
47	Efficient viscosity contrast calculation for blood flow simulations using the lattice Boltzmann method. International Journal for Numerical Methods in Fluids, 2020, 92, 1463-1477.	0.9	8
48	Machine learning for condensed matter physics. Journal of Physics Condensed Matter, 2021, 33, 053001.	0.7	47
49	PyOIF: Computational tool for modelling of multi-cell flows in complex geometries. PLoS Computational Biology, 2020, 16, e1008249.	1.5	15
50	Computer Simulations of Dynamic Response of Ferrofluids on an Alternating Magnetic Field with High Amplitude. Mathematics, 2021, 9, 2581.	1.1	3
51	The influence of polydispersity on the structural properties of the isotropic phase of magnetic nanoplatelets. Journal of Molecular Liquids, 2020, 312, 113293.	2.3	5
52	The numerical investigation of magnetic properties of metal-oxide based nanofluid. , 2021, , .		0
53	Tunable Knot Segregation in Copolyelectrolyte Rings Carrying a Neutral Segment. ACS Macro Letters, 2021, 10, 1365-1370.	2.3	5
54	Magnetostriction in elastomers with mixtures of magnetically hard and soft microparticles: effects of nonlinear magnetization and matrix rigidity. ChemistrySelect, 2022, 7, 1187-1208.	0.7	3

#	Article	IF	Citations
56	Trilateration-Based Multilevel Method for Minimizing the Lennard-Jones Potential. Lecture Notes in Computer Science, 2020, , 163-175.	1.0	0
57	Computational study of inertial effects in toroidal and helical microchannels. , 2020, , .		0
58	Proof-of-concept model of red blood cell with coarse-grained hemoglobin. , 2020, , .		0
59	Behaviour of a magnetic nanogel in a shear flow. Journal of Molecular Liquids, 2022, 346, 118056.	2.3	6
61	DPD Modelling of the Self- and Co-Assembly of Polymers and Polyelectrolytes in Aqueous Media: Impact on Polymer Science. Polymers, 2022, 14, 404.	2.0	16
62	Machine learning classification of trajectories from molecular dynamics simulations of chromosome segregation. PLoS ONE, 2022, 17, e0262177.	1.1	1
63	Magneto-elastic coupling as a key to microstructural response of magnetic elastomers with flake-like particles. Soft Matter, 2022, 18, 496-506.	1.2	7
64	Simulation of Shape and Structure Response of Nonspherical Magnetosensitive Vesicles Subjected to Magnetic Fields. IEEE Magnetics Letters, 2022, 13, 1-5.	0.6	0
65	Capture and translocation of a rod-like molecule by a nanopore: orientation, charge distribution and hydrodynamics. Physical Chemistry Chemical Physics, 2022, 24, 6444-6452.	1.3	3
66	Energetically favorable configurations of hematite cube chains. Physical Review E, 2022, 105, 024605.	0.8	3
67	The pH-Dependent Swelling of Weak Polyelectrolyte Hydrogels Modeled at Different Levels of Resolution. Macromolecules, 2022, 55, 3176-3188.	2.2	11
68	The primitive model in classical density functional theory: beyond the standard mean-field approximation. Journal of Physics Condensed Matter, 2022, 34, 235101.	0.7	5
69	Mild stratification in drying films of colloidal mixtures. Soft Matter, 2022, 18, 3487-3497.	1.2	6
70	Analytical and computational study of cascade reaction processes in catalytic fibrous membranes. Computers and Fluids, 2022, , 105438.	1.3	0
71	The importance of being a cube: active cubes in a microchannel. Journal of Molecular Liquids, 2022, , 119318.	2.3	0
72	Structural and magnetic equilibrium properties of a semi-dilute suspension of magnetic multicore nanoparticles. Journal of Molecular Liquids, 2022, 359, 119373.	2.3	5
73	Organized states arising from compression of single semiflexible polymer chains in nanochannels. Physical Review E, 2022, 105, .	0.8	3
74	A Transfer Free Energy Based Implicit Solvent Model for Protein Simulations in Solvent Mixtures: Urea-Induced Denaturation as a Case Study. Journal of Physical Chemistry B, 2022, 126, 4472-4482.	1.2	3

#	Article	IF	Citations
75	An empirical method to characterize displacement distribution functions for anomalous and transient diffusion. Physica A: Statistical Mechanics and Its Applications, 2022, 604, 127676.	1.2	0
76	Contact area of cell cluster in a simple bifurcation. , 2022, , .		1
78	A thermalized electrokinetics model including stochastic reactions suitable for multiscale simulations of reactionâ€“advectionâ€“diffusion systems. Journal of Computational Science, 2022, 63, 101770.	1.5	4
79	Fluid-Gel Coexistence in Lipid Membranes under Differential Stress. Biophysical Journal, 2022, , .	0.2	3
80	Distribution of cholesterol in asymmetric membranes driven by composition and differential stress. Biophysical Journal, 2022, 121, 4001-4018.	0.2	22
81	Towards Nematic Phases in Ionic Liquid Crystals â€“ A Simulation Study. ChemPhysChem, 2023, 24, .	1.0	6
82	Simulations Explain the Swelling Behavior of Hydrogels with Alternating Neutral and Weakly Acidic Blocks. Macromolecules, 2022, 55, 10751-10760.	2.2	9
83	Optimising nanoporous supercapacitors for heat-to-electricity conversion. Journal of Molecular Liquids, 2023, 371, 121093.	2.3	4
84	Tuning Knotted Copolyelectrolyte Conformations via Solution Properties. Macromolecules, 2022, 55, 10761-10772.	2.2	1
85	Modeling cell clusters and their near-wall dynamics in shear flow. Computational Particle Mechanics, 0, , .	1.5	0
86	Interplay between steric and hydrodynamic interactions for ellipsoidal magnetic nanoparticles in a polymer suspension. Soft Matter, 2023, 19, 1186-1193.	1.2	2
88	Ratcheting Charged Polymers through Symmetric Nanopores Using Pulsed Fields: Designing a Low Pass Filter for Concentrating Polyelectrolytes. Nano Letters, 2023, 23, 1343-1349.	4.5	2
89	Coarse-Grained Molecular Simulation of Extracellular Vesicles Squeezing for Drug Loading. Physical Chemistry Chemical Physics, 0, , .	1.3	1
90	Implicit-Solvent Coarse-Grained Simulations of Linearâ€“Dendritic Block Copolymer Micelles. International Journal of Molecular Sciences, 2023, 24, 2763.	1.8	2
91	Rectification of polymer translocation through nanopores by nonchiral and chiral active particles. Physical Review E, 2023, 107, .	0.8	2
92	MDSuite: comprehensive post-processing tool for particle simulations. Journal of Cheminformatics, 2023, 15, .	2.8	0
93	Anomalous Underscreening in the Restricted Primitive Model. Physical Review Letters, 2023, 130, .	2.9	12
94	Modeling the Phase Transition in Hydrophobic Weak Polyelectrolyte Gels under Compression. Gels, 2023, 9, 259.	2.1	1

#	Article	IF	Citations
95	Molecular Dynamics Simulations of Ionic Liquid Crystals. , 2024, , 723-761.		1
98	Cluster formation in microferrogels: Dependence on the network crosslink density and the character of magnetic nanoparticle distribution. AIP Conference Proceedings, 2023, , .	0.3	0
100	ESPResSo, a Versatile Open-Source Software Package for Simulating Soft Matter Systems. , 2024, , 578-601.		1
104	Simulation of the small ferrogel sample with an implementation of the Lennard-Jones fluid model. AIP Conference Proceedings, 2023, , .	0.3	0
113	State of the Practice for Lattice Boltzmann Method Software. Archives of Computational Methods in Engineering, 0, , .	6.0	0