Christian Holm

List of Publications by Year
in descending order

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293 papers	12,729 citations	20759 60 h-index	38300 95 g-index
316 all docs	316 docs citations	316 times ranked	7378 citing authors

#	Article	IF	Citations
1	ESPResSoâ€"an extensible simulation package for research on soft matter systems. Computer Physics Communications, 2006, 174, 704-727.	3.0	612
2	How to mesh up Ewald sums. I. A theoretical and numerical comparison of various particle mesh routines. Journal of Chemical Physics, 1998, 109, 7678-7693.	1.2	576
3	How to mesh up Ewald sums. II. An accurate error estimate for the particleâ€"particleâ€"particle-mesh algorithm. Journal of Chemical Physics, 1998, 109, 7694-7701.	1.2	284
4	Fraction of Condensed Counterions around a Charged Rod:Â Comparison of Poissonâ^'Boltzmann Theory and Computer Simulations. Macromolecules, 2000, 33, 199-206.	2.2	271
5	Force Fields for Studying the Structure and Dynamics of Ionic Liquids: A Critical Review of Recent Developments. ChemPhysChem, 2012, 13, 1625-1637.	1.0	239
6	Strongly Charged, Flexible Polyelectrolytes in Poor Solvents:Â Molecular Dynamics Simulationsâ€. Langmuir, 1999, 15, 4033-4044.	1.6	219
7	The structure of ferrofluids: A status report. Current Opinion in Colloid and Interface Science, 2005, 10, 133-140.	3.4	214
8	Molecular dynamics study on the equilibrium magnetization properties and structure of ferrofluids. Physical Review E, 2002, 66, 021405.	0.8	206
9	Critical exponents of the classical three-dimensional Heisenberg model: A single-cluster Monte Carlo study. Physical Review B, 1993, 48, 936-950.	1.1	192
10	Electrostatics in periodic slab geometries. I. Journal of Chemical Physics, 2002, 117, 2496-2502.	1.2	144
11	Polyelectrolyte Theory. Advances in Polymer Science, 0, , 67-111.	0.4	140
12	Single-Chain Properties of Polyelectrolytes in Poor Solventâ€. Journal of Physical Chemistry B, 2003, 107, 8041-8055.	1.2	135
13	Osmotic coefficients of atomistic NaCl (aq) force fields. Journal of Chemical Physics, 2006, 124, 164509.	1.2	132
14	Magnetic properties of polydisperse ferrofluids: A critical comparison between experiment, theory, and computer simulation. Physical Review E, 2007, 75, 061405.	0.8	130
15	Strong Attraction between Charged Spheres due to Metastable Ionized States. Physical Review Letters, 2000, 85, 872-875.	2.9	127
16	Structure and magnetic properties of polydisperse ferrofluids: A molecular dynamics study. Physical Review E, 2003, 68, 041401.	0.8	127
17	ESPResSo 4.0 â€" an extensible software package for simulating soft matter systems. European Physical Journal: Special Topics, 2019, 227, 1789-1816.	1.2	127
18	Modeling the separation of macromolecules: A review of current computer simulation methods. Electrophoresis, 2009, 30, 792-818.	1.3	126

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19	ESPResSo 3.1: Molecular Dynamics Software for Coarse-Grained Models. Lecture Notes in Computational Science and Engineering, 2013, , 1-23.	0.1	118
20	Overcharging of DNA in the Presence of Salt:Â Theory and Simulation. Journal of Physical Chemistry B, 2001, 105, 10983-10991.	1.2	117
21	Electrophoresis of Colloidal Dispersions in the Low-Salt Regime. Physical Review Letters, 2007, 98, 176105.	2.9	114
22	Ionic Charge Reduction and Atomic Partial Charges from First-Principles Calculations of 1,3-Dimethylimidazolium Chloride. Journal of Physical Chemistry B, 2010, 114, 6150-6155.	1.2	113
23	Effect of Anions on Static Orientational Correlations, Hydrogen Bonds, and Dynamics in Ionic Liquids:â€‰ A Simulational Study. Journal of Physical Chemistry B, 2008, 112, 1743-1751.	1.2	111
24	Modeling Multibody Effects in Ionic Solutions with a Concentration Dependent Dielectric Permittivity. Physical Review Letters, 2006, 96, 147801.	2.9	110
25	Optimizing working parameters of the smooth particle mesh Ewald algorithm in terms of accuracy and efficiency. Journal of Chemical Physics, 2010, 133, 034117.	1.2	108
26	Estimate of the cutoff errors in the Ewald summation for dipolar systems. Journal of Chemical Physics, 2001, 115, 6351-6359.	1.2	105
27	Machine-learned interatomic potentials by active learning: amorphous and liquid hafnium dioxide. Npj Computational Materials, 2020, 6, .	3.5	100
28	Ionic liquids studied across different scales: A computational perspective. Faraday Discussions, 2012, 154, 111-132.	1.6	99
29	Ionic screening and dissociation are crucial for understanding chemical self-propulsion in polar solvents. Soft Matter, 2017, 13, 1200-1222.	1.2	95
30	Locality and Fluctuations: Trends in Imidazolium-Based Ionic Liquids and Beyond. Journal of Chemical Theory and Computation, 2011, 7, 3040-3044.	2.3	93
31	Structure of polyelectrolytes in poor solvent. Europhysics Letters, 2002, 60, 566-572.	0.7	92
32	Swelling of polyelectrolyte networks. Journal of Chemical Physics, 2005, 122, 154903.	1.2	92
33	Overcharging: The crucial role of excluded volume. Europhysics Letters, 2002, 60, 383-389.	0.7	89
34	A comparative study of two classical force fields on statics and dynamics of [EMIM][BF4] investigated via molecular dynamics simulations. Journal of Chemical Physics, 2008, 129, 224501.	1.2	89
35	Deformation mechanisms in 2D magnetic gels studied by computer simulations. Soft Matter, 2012, 8, 9923.	1.2	87
36	P 3 M algorithm for dipolar interactions. Journal of Chemical Physics, 2008, 129, 234104.	1.2	84

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37	Importance of Hydrodynamic Shielding for the Dynamic Behavior of Short Polyelectrolyte Chains. Physical Review Letters, 2008, 100, 096104.	2.9	82
38	Charge Me Slowly, I Am in a Hurry: Optimizing Chargeâ€“Discharge Cycles in Nanoporous Supercapacitors. ACS Nano, 2018, 12, 9733-9741.	7.3	80
39	Simulations of ionization equilibria in weak polyelectrolyte solutions and gels. Soft Matter, 2019, 15, 1155-1185.	1.2	78
40	A stable local density functional approach to ion-ion correlations. Europhysics Letters, 2000, 52, 80-86.	0.7	76
41	Attraction and Ionic Correlations between Charged Stiff Polyelectrolytes. Macromolecules, 2003, 36, 249-259.	2.2	76
42	An iterative, fast, linear-scaling method for computing induced charges on arbitrary dielectric boundaries. Journal of Chemical Physics, 2010, 132, 154112.	1.2	76
43	Polyelectrolyte Multilayering on a Charged Sphere. Langmuir, 2003, 19, 4473-4482.	1.6	75
44	Electrostatics in periodic slab geometries. II. Journal of Chemical Physics, 2002, 117, 2503-2512.	1.2	73
45	MMM2D: A fast and accurate summation method for electrostatic interactions in 2D slab geometries. Computer Physics Communications, 2002, 148, 327-348.	3.0	73
46	Incorporation of excluded-volume correlations into Poisson-Boltzmann theory. Physical Review E, 2005, 71, 061106.	0.8	73
47	Polymer architecture of magnetic gels: a review. Journal of Physics Condensed Matter, 2018, 30, 063002.	0.7	73
48	Electrophoretic mobility of a charged colloidal particle: a computer simulation study. Journal of Physics Condensed Matter, 2004, 16, S4063-S4073.	0.7	72
49	Comparison of scalable fast methods for long-range interactions. Physical Review E, 2013, 88, 063308.	0.8	72
50	Modeling of Polyelectrolyte Gels in Equilibrium with Salt Solutions. Macromolecules, 2015, 48, 7698-7708.	2.2	72
51	Capacitance of Nanoporous Carbon-Based Supercapacitors Is a Trade-Off between the Concentration and the Separability of the Ions. Journal of Physical Chemistry Letters, 2016, 7, 4015-4021.	2.1	72
52	Comparison of a hydrogel model to the Poissonâ€“Boltzmann cell model. Journal of Chemical Physics, 2009, 131, 094903.	1.2	69
53	Coarse-grained simulations of polyelectrolyte complexes: MARTINI models for poly(styrene sulfonate) and poly(diallyldimethylammonium). Journal of Chemical Physics, 2015, 143, 243151.	1.2	69
54	A refined polarizable water model for the coarse-grained MARTINI force field with long-range electrostatic interactions. Journal of Chemical Physics, 2017, 146, 054501.	1.2	69

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55	Buckling of paramagnetic chains in soft gels. Soft Matter, 2016, 12, 228-237.	1.2	68
56	Strong electrostatic interactions in spherical colloidal systems. Physical Review E, 2001, 64, 021405.	0.8	66
57	Scaling in polyelectrolyte networks. Europhysics Letters, 2004, 67, 786-792.	0.7	64
58	Computer simulations of the structure of colloidal ferrofluids. Physical Review E, 2005, 71, 061203.	0.8	64
59	Ground state structures in ferrofluid monolayers. Physical Review E, 2009, 80, 031404.	0.8	64
60	Electrophoretic mobility and charge inversion of a colloidal particle studied by single-colloid electrophoresis and molecular dynamics simulations. Physical Review E, 2013, 87, 022302.	0.8	64
61	End effects of strongly charged polyelectrolytes: A molecular dynamics study. Journal of Chemical Physics, 2001, 114, 9674-9682.	1.2	63
62	Concentration dependent effects of urea binding to poly(N-isopropylacrylamide) brushes: a combined experimental and numerical study. Physical Chemistry Chemical Physics, 2016, 18, 5324-5335.	1.3	61
63	Polyelectrolytes in electric fields: measuring the dynamical effective charge and effective friction. Soft Matter, 2009, 5, 2079.	1.2	58
64	How to speed up ion transport in nanopores. Nature Communications, 2020, 11, 6085.	5.8	57
65	Understanding polyelectrolyte multilayers: an open challenge for simulations. Soft Matter, 2009, 5, 4412.	1.2	54
66	Electrode Models for Ionic Liquid-Based Capacitors. Journal of Physical Chemistry C, 2015, 119, 22445-22451.	1.5	54
67	Attraction and unbinding of like-charged rods. Europhysics Letters, 2004, 67, 130-136.	0.7	53
68	Applying the chain formation model to magnetic properties of aggregated ferrofluids. Physical Review E, 2004, 69, 031206.	0.8	52
69	Origin of Current Blockades in Nanopore Translocation Experiments. Physical Review Letters, 2014, 112, 018101.	2.9	51
70	Finite-size scaling study of the three-dimensional classical Heisenberg model. Physics Letters, Section A: General, Atomic and Solid State Physics, 1993, 173, 8-12.	0.9	50
71	Microstructure analysis of monodisperse ferrofluid monolayers: theory and simulation. Physical Chemistry Chemical Physics, 2008, 10, 1883.	1.3	50
72	Towards multiscale modeling of ionic liquids: From electronic structure to bulk properties. Journal of Molecular Liquids, 2010, 152, 2-8.	2.3	50

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73	Complex Tracer Diffusion Dynamics in Polymer Solutions. Physical Review Letters, 2013, 111, 088301.	2.9	50
74	The osmotic coefficient of rod-like polyelectrolytes: Computer simulation, analytical theory, and experiment. European Physical Journal E, 2001, 5, 97-103.	0.7	49
75	The Swelling Behavior of Charged Hydrogels. Macromolecular Symposia, 2006, 237, 90-107.	0.4	48
76	Mesoscopic simulations of the counterion-induced electro-osmotic flow: A comparative study. Journal of Chemical Physics, 2009, 130, 244702.	1.2	48
77	Ferrogels cross-linked by magnetic nanoparticlesâ€"Deformation mechanisms in two and three dimensions studied by means of computer simulations. Journal of Magnetism and Magnetic Materials, 2015, 383, 262-266.	1.0	48
78	Peptides in the presence of aqueous ionic liquids: tunable co-solutes as denaturants or protectants?. Physical Chemistry Chemical Physics, 2015, 17, 26049-26053.	1.3	48
79	Effect of colloidal charge discretization in the primitive model. European Physical Journal E, 2001, 4, 363-370.	0.7	47
80	Stiff-Chain Polyelectrolytes. Advances in Polymer Science, 0, , 1-27.	0.4	47
81	Ferrofluids with shifted dipoles: ground state structures. Soft Matter, 2011, 7, 5217.	1.2	46
82	Microfluidic pumping by micromolar salt concentrations. Soft Matter, 2017, 13, 1505-1518.	1.2	46
83	Poly(styrenesulfonate)â^'Poly(diallyldimethylammonium) Mixtures: Toward the Understanding of Polyelectrolyte Complexes and Multilayers via Atomistic Simulations. Macromolecules, 2010, 43, 7828-7838.	2.2	45
84	Conformational properties of poor solvent polyelectrolytes. Computer Physics Communications, 2002, 147, 321-324.	3.0	44
85	Hydrogels in Poor Solvents: A Molecular Dynamics Study. Macromolecular Theory and Simulations, 2011, 20, 721-734.	0.6	44
86	Grand-Reaction Method for Simulations of Ionization Equilibria Coupled to Ion Partitioning. Macromolecules, 2020, 53, 3007-3020.	2.2	44
87	High-temperature series analyses of the classical Heisenberg and XY models. Physica A: Statistical Mechanics and Its Applications, 1993, 201, 581-592.	1.2	43
88	Electrostatic layer correction with image charges: A linear scaling method to treat slab 2D+h systems with dielectric interfaces. Journal of Chemical Physics, 2008, 129, 204102.	1.2	43
89	Theory and simulations of rigid polyelectrolytes. Molecular Physics, 2002, 100, 2941-2956.	0.8	41
90	Simulation of charge reversal in salty environments: Giant overcharging?. European Physical Journal E, 2008, 26, 191-195.	0.7	41

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91	Efficient Algorithms for Electrostatic Interactions Including Dielectric Contrasts. Entropy, 2013, 15, 4569-4588.	1.1	41
92	Electrolyte solvents for high voltage lithium ion batteries: ion correlation and specific anion effects in adiponitrile. Physical Chemistry Chemical Physics, 2018, 20, 25701-25715.	1.3	41
93	A novel method for calculating electrostatic interactions in 2D periodic slab geometries. Chemical Physics Letters, 2002, 354, 324-330.	1.2	40
94	Boundary condition effects in the simulation study of equilibrium properties of magnetic dipolar fluids. Journal of Chemical Physics, 2003, 119, 379-387.	1.2	40
95	Equilibrium properties of a bidisperse ferrofluid with chain aggregates: theory and computer simulations. Journal of Physics Condensed Matter, 2006, 18, S2737-S2756.	0.7	40
96	The solvation and ion condensation properties for sulfonated polyelectrolytes in different solventsâ€"a computational study. New Journal of Physics, 2014, 16, 025001.	1.2	40
97	Ferrogels cross-linked by magnetic particles: Field-driven deformation and elasticity studied using computer simulations. Journal of Chemical Physics, 2015, 143, 154901.	1.2	40
98	The raspberry model for hydrodynamic interactions revisited. I. Periodic arrays of spheres and dumbbells. Journal of Chemical Physics, 2015, 143, 084107.	1.2	40
99	Solvent effects of 1-ethyl-3-methylimidazolium acetate: solvation and dynamic behavior of polar and apolar solutes. Physical Chemistry Chemical Physics, 2015, 17, 8480-8490.	1.3	40
100	Lattice-Boltzmann hydrodynamics of anisotropic active matter. Journal of Chemical Physics, 2016, 144, 134106.	1.2	40
101	Simulation of weak polyelectrolytes: a comparison between the constant pH and the reaction ensemble method. European Physical Journal: Special Topics, 2017, 226, 725-736.	1.2	40
102	MMM1D: A method for calculating electrostatic interactions in one-dimensional periodic geometries. Journal of Chemical Physics, 2005, 123, 144103.	1.2	39
103	Tail-induced attraction between nucleosome core particles. Physical Review E, 2006, 74, 031919.	0.8	39
104	DFT Accurate Interatomic Potential for Molten NaCl from Machine Learning. Journal of Physical Chemistry C, 2020, 124, 25760-25768.	1.5	39
105	Polyelectrolyte adsorption and multilayering on charged colloidal particles. Journal of Polymer Science, Part B: Polymer Physics, 2004, 42, 3557-3570.	2.4	38
106	Electrostatic properties of liquid 1,3-dimethylimidazolium chloride: role of local polarization and effect of the bulk. Physical Chemistry Chemical Physics, 2010, 12, 1817-1821.	1.3	38
107	How close to two dimensions does a Lennard-Jones system need to be to produce a hexatic phase?. Journal of Chemical Physics, 2011, 135, 054514.	1.2	38
108	Like-charge colloidâ€"polyelectrolyte complexation. Journal of Chemical Physics, 2002, 117, 2947-2960.	1.2	37

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109	Monte Carlo study of topological defects in the 3D Heisenberg model. Journal of Physics A, 1994, 27, 2553-2563.	1.6	36
110	Ground state of two unlike charged colloids: An analogy with ionic bonding. Europhysics Letters, 2000, 51, 461-467.	0.7	36
111	ICMMM2D: An accurate method to include planar dielectric interfaces via image charge summation. Journal of Chemical Physics, 2007, 127, 154723.	1.2	36
112	Finite-size polyelectrolyte bundles at thermodynamic equilibrium. Europhysics Letters, 2007, 77, 16001.	0.7	35
113	A self-consistent mean-field model for polyelectrolyte gels. Soft Matter, 2017, 13, 3264-3274.	1.2	34
114	Study of 1,3-dimethylimidazolium chloride with electronic structure methods and force field approaches. Journal of Chemical Physics, 2008, 129, 174503.	1.2	33
115	Shear effects on crystal nucleation in colloidal suspensions. Physical Review E, 2008, 78, 031403.	0.8	33
116	Atomistic Study of Surface Effects on Polyelectrolyte Adsorption: Case Study of a Poly(styrenesulfonate) Monolayer. Macromolecules, 2011, 44, 1707-1718.	2.2	33
117	Importance of Varying Permittivity on the Conductivity of Polyelectrolyte Solutions. Physical Review Letters, 2015, 115, 118301.	2.9	33
118	On the efficiency of a hydrogel-based desalination cycle. Desalination, 2017, 414, 28-34.	4.0	33
119	The critical behaviour of Ising spins on 2D Regge lattices. Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics, 1994, 335, 143-150.	1.5	32
120	Cluster formation in systems of shifted-dipole particles. Soft Matter, 2013, 9, 3535.	1.2	32
121	Generic force fields for ionic liquids. Journal of Molecular Liquids, 2014, 192, 32-37.	2.3	32
122	Local Water Dynamics around Antifreeze Protein Residues in the Presence of Osmolytes: The Importance of Hydroxyl and Disaccharide Groups. Journal of Physical Chemistry B, 2014, 118, 11613-11621.	1.2	32
123	A polarizable MARTINI model for monovalent ions in aqueous solution. Journal of Chemical Physics, 2018, 149, 163319.	1.2	32
124	Controlled DNA compaction within chromatin: The tail-bridging effect. Europhysics Letters, 2006, 73, 135-141.	0.7	31
125	Simulational study of anomalous tracer diffusion in hydrogels. Colloid and Polymer Science, 2011, 289, 523-534.	1.0	31
126	Dynamics in Stimuli-Responsive Poly(N-isopropylacrylamide) Hydrogel Layers As Revealed by Fluorescence Correlation Spectroscopy. Macromolecules, 2014, 47, 5303-5312.	2.2	31

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127	Aggregate formation in ferrofluid monolayers: simulations and theory. Journal of Physics Condensed Matter, 2008, 20, 204125.	0.7	30
128	Behavior of bulky ferrofluids in the diluted low-coupling regime: Theory and simulation. Physical Review E, 2010, 81, 011501.	0.8	30
129	Influence of Charged Polymer Coatings on Electro-Osmotic Flow: Molecular Dynamics Simulations. Macromolecules, 2011, 44, 9455-9463.	2.2	30
130	Preferential solvation and ion association properties in aqueous dimethyl sulfoxide solutions. Physical Chemistry Chemical Physics, 2016, 18, 31312-31322.	1.3	30
131	Bulk ionic screening lengths from extremely large-scale molecular dynamics simulations. Chemical Communications, 2020, 56, 15635-15638.	2.2	30
132	Cell Model and Poisson-Boltzmann Theory: A Brief Introduction. , 2001, , 27-52.		30
133	Efficient Methods to Compute Long-Range Interactions for Soft Matter Systems. , 0, , 59-109.		29
134	Optimal Cell Approach to Osmotic Properties of Finite Stiff-Chain Polyelectrolytes. Physical Review Letters, 2006, 96, 088302.	2.9	29
135	Colloidal electrophoresis: scaling analysis, Greenâ€“Kubo relation, and numerical results. Journal of Physics Condensed Matter, 2008, 20, 404214.	0.7	29
136	How to analyse the structure factor in ferrofluids with strong magnetic interactions: a combined analytic and simulation approach. Molecular Physics, 2009, 107, 571-590.	0.8	29
137	Mobility Reversal of Polyelectrolyte-Grafted Colloids in Monovalent Salt Solutions. Physical Review Letters, 2014, 113, 238301.	2.9	29
138	Simulation of electric double layers around charged colloids in aqueous solution of variable permittivity. Journal of Chemical Physics, 2014, 141, 064902.	1.2	29
139	Diffusiophoretic Self-Propulsion for Partially Catalytic Spherical Colloids. IEEE Transactions on Nanobioscience, 2015, 14, 272-288.	2.2	29
140	The effect of finite pore length on ion structure and charging. Journal of Chemical Physics, 2017, 147, 104708.	1.2	29
141	Mesoscale modelling of polyelectrolyteelectrophoresis. Faraday Discussions, 2010, 144, 57-70.	1.6	28
142	Effects of the dipolar interaction on the equilibrium morphologies of a single supramolecular magnetic filament in bulk. Journal of Chemical Physics, 2013, 139, 044904.	1.2	28
143	Properties of Apolar Solutes in Alkyl Imidazoliumâ€Based Ionic Liquids: The Importance of Local Interactions. ChemPhysChem, 2016, 17, 387-394.	1.0	28
144	Poly(sodium acrylate) hydrogels: synthesis of various network architectures, local molecular dynamics, salt partitioning, desalination and simulation. Soft Matter, 2019, 15, 9949-9964.	1.2	28

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145	Specific ion effects for polyelectrolytes in aqueous and non-aqueous media: the importance of the ion solvation behavior. Soft Matter, 2018, 14, 6243-6255.	1.2	27
146	Ensemble inequivalence in single-molecule experiments. Physical Review E, 2009, 79, 051118.	0.8	26
147	Interlaced P3M algorithm with analytical and ik-differentiation. Journal of Chemical Physics, 2010, 132, 234103.	1.2	26
148	Phase diagram for a single flexible Stockmayer polymer at zero field. Soft Matter, 2013, 9, 7185.	1.2	26
149	The Raspberry model for hydrodynamic interactions revisited. II. The effect of confinement. Journal of Chemical Physics, 2015, 143, 084108.	1.2	26
150	First-Principles Parametrization of Polarizable Coarse-Grained Force Fields for Ionic Liquids. Journal of Chemical Theory and Computation, 2018, 14, 1471-1486.	2.3	26
151	Polyelectrolyte bundles. Journal of Physics Condensed Matter, 2004, 16, S2135-S2144.	0.7	25
152	Communication: Kinetic and pairing contributions in the dielectric spectra of electrolyte solutions. Journal of Chemical Physics, 2014, 140, 211101.	1.2	25
153	Coarse-grained simulations of an ionic liquid-based capacitor: I. Density, ion size, and valency effects. Journal of Physics Condensed Matter, 2014, 26, 284108.	0.7	25
154	Towards a scale-bridging description of ferrogels and magnetic elastomers. Journal of Physics Condensed Matter, 2015, 27, 325105.	0.7	25
155	Properties of the polarizable MARTINI water model: A comparative study for aqueous electrolyte solutions. Journal of Molecular Liquids, 2015, 212, 103-110.	2.3	25
156	Understanding the onset of oscillatory swimming in microchannels. Soft Matter, 2016, 12, 4704-4708.	1.2	25
157	Hyperspin manifolds. International Journal of Theoretical Physics, 1986, 25, 441-463.	0.5	24
158	A lattice Boltzmann model for squirmers. Journal of Chemical Physics, 2019, 150, 144110.	1.2	24
159	Osmotic Coefficient Calculations for Dilute Solutions of Short Stiff-Chain Polyelectrolytes. Macromolecules, 2007, 40, 731-738.	2.2	23
160	The optimal P3M algorithm for computing electrostatic energies in periodic systems. Journal of Chemical Physics, 2008, 128, 034109.	1.2	23
161	Refining classical force fields for ionic liquids: theory and application to [MMIM][Cl]. Physical Chemistry Chemical Physics, 2013, 15, 2037-2049.	1.3	23
162	Microstructure and magnetic properties of magnetic fluids consisting of shifted dipole particles under the influence of an external magnetic field. Journal of Chemical Physics, 2013, 139, 214901.	1.2	23

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163	Moving charged particles in lattice Boltzmann-based electrokinetics. Journal of Chemical Physics, 2016, 145, 214102.	1.2	23
164	Microphase separation and the formation of ion conductivity channels in poly(ionic liquid)s: A coarse-grained molecular dynamics study. Journal of Chemical Physics, 2018, 148, 193824.	1.2	23
165	Studying the field-controlled change of shape and elasticity of magnetic gels using particle-based simulations. Archive of Applied Mechanics, 2019, 89, 3-16.	1.2	23
166	An extensible lattice Boltzmann method for viscoelastic flows: complex and moving boundaries in Oldroyd-B fluids. European Physical Journal E, 2021, 44, 1.	0.7	23
167	Implicit Method for Simulating Electrohydrodynamics of Polyelectrolytes. Physical Review Letters, 2010, 105, 148301.	2.9	22
168	Equilibrium polyelectrolyte bundles with different multivalent counterion concentrations. Physical Review E, 2010, 82, 031901.	0.8	22
169	Magnetic particles with shifted dipoles. Journal of Magnetism and Magnetic Materials, 2011, 323, 1269-1272.	1.0	22
170	Influence of Cosolutes on Chemical Equilibrium: a Kirkwoodâ€“Buff Theory for Ion Pair Associationâ€“Dissociation Processes in Ternary Electrolyte Solutions. Journal of Physical Chemistry C, 2018, 122, 10293-10302.	1.5	22
171	Hydrodynamic mobility reversal of squirmers near flat and curved surfaces. Soft Matter, 2019, 15, 5908-5920.	1.2	22
172	Structure and magnetic properties of mono- and bi-dispersed ferrofluids as revealed by simulations. Journal of Magnetism and Magnetic Materials, 2005, 289, 234-237.	1.0	21
173	An atomistic study of a poly(styrene sulfonate)/poly(diallyldimethylammonium) bilayer: the role of surface properties and charge reversal. Physical Chemistry Chemical Physics, 2011, 13, 16336.	1.3	21
174	How to Convert SPME to P3M: Influence Functions and Error Estimates. Journal of Chemical Theory and Computation, 2012, 8, 936-947.	2.3	21
175	Tracer diffusion in a crowded cylindrical channel. Physical Review E, 2013, 87, 062709.	0.8	21
176	Coarse-grained molecular dynamics simulation of small ferrogel objects. Journal of Magnetism and Magnetic Materials, 2015, 383, 277-280.	1.0	21
177	Reducing spurious flow in simulations of electrokinetic phenomena. Journal of Chemical Physics, 2016, 145, 044901.	1.2	21
178	The efficiency of self-phoretic propulsion mechanisms with surface reaction heterogeneity. Journal of Chemical Physics, 2016, 144, 204902.	1.2	21
179	Conformation of a polyelectrolyte complexed to a like-charged colloid. Physical Review E, 2002, 65, 041805.	0.8	20
180	Spatial distribution of polyelectrolyte and counterions in nanocapsules: A computer simulation study. Physical Review E, 2006, 73, 021801.	0.8	20

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181	Electrophoresis of a Spherical Polyelectrolyte-Grafted Colloid in Monovalent Salt Solutions: Comparison of Molecular Dynamics Simulations with Theory and Numerical Calculations. Macromolecules, 2015, 48, 775-787.	2.2	20
182	Order and information in the patterns of spinning magnetic micro-disks at the air-water interface. Science Advances, 2022, 8, eabk0685.	4.7	20
183	Ising spins on a gravitating sphere. Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics, 1996, 375, 69-74.	1.5	19
184	Conformations and solution structure of polyelectrolytes in poor solvent. Macromolecular Symposia, 2004, 211, 43-54.	0.4	19
185	Applying to DNA translocation: Effect of dielectric boundaries. Computer Physics Communications, 2011, 182, 33-35.	3.0	19
186	Toward Understanding of Self-Electrophoretic Propulsion under Realistic Conditions: From Bulk Reactions to Confinement Effects. Accounts of Chemical Research, 2018, 51, 2998-3005.	7.6	19
187	Ionic screening in bulk and under confinement. Journal of Chemical Physics, 2021, 155, 204501.	1.2	19
188	Computer Simulations of the â€œHairy Rodâ€•Model. Macromolecular Chemistry and Physics, 2005, 206, 77-82.	1.1	18
189	Computing the Electrophoretic Mobility of Large Spherical Colloids by Combining Explicit Ion Simulations with the Standard Electrokinetic Model. Langmuir, 2014, 30, 1758-1767.	1.6	18
190	Permeability Estimation of Regular Porous Structures: A Benchmark for Comparison of Methods. Transport in Porous Media, 2021, 138, 1-23.	1.2	18
191	Critical Exponents of the Classical Heisenberg Ferromagnet. Physical Review Letters, 1997, 78, 2265-2265.	2.9	17
192	Coarse-grained simulations of an ionic liquid-based capacitor: II. Asymmetry in ion shape and charge localization. Journal of Physics Condensed Matter, 2014, 26, 284114.	0.7	17
193	Wangâ€“Landau Reaction Ensemble Method: Simulation of Weak Polyelectrolytes and General Acidâ€“Base Reactions. Journal of Chemical Theory and Computation, 2017, 13, 852-862.	2.3	17
194	Computer Simulations of Static and Dynamical Properties of Weak Polyelectrolyte Nanogels in Salty Solutions. Gels, 2018, 4, 2.	2.1	17
195	The Effect of Small Organic Cosolutes on Water Structure and Dynamics. Journal of Chemical & Engineering Data, 2020, 65, 1197-1210.	1.0	17
196	Frequency-dependent magnetic susceptibility of magnetic nanoparticles in a polymer solution: a simulation study. Soft Matter, 2021, 17, 174-183.	1.2	17
197	Semiflexible magnetic filaments near attractive flat surfaces: a Langevin dynamics study. Soft Matter, 2011, 7, 1809-1818.	1.2	16
198	Lattice-Boltzmann simulations of the electrophoretic stretching of polyelectrolytes: The importance of hydrodynamic interactions. Journal of Chemical Physics, 2014, 140, 164904.	1.2	16

#	Article	IF	Citations
199	A coarse-grained polarizable force field for the ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate. Journal of Physics Condensed Matter, 2017, 29, 504004.	0.7	16
200	Charge inversion in colloidal systems. Computer Physics Communications, 2002, 147, 282-285.	3.0	15
201	Magnetization of polydisperse colloidal ferrofluids: Effect of magnetostriction. Physical Review E, 2004, 70, 061404.	0.8	15
202	Stretching of surface-tethered polymers in pressure-driven flow under confinement. Soft Matter, 2017, 13, 6189-6196.	1.2	15
203	Electrostatically Cross-Linked Reversible Gelsâ€"Effects of pH and Ionic Strength. Macromolecules, 2021, 54, 4769-4781.	2.2	15
204	Highly Efficient Active Colloids Driven by Galvanic Exchange Reactions. Journal of the American Chemical Society, 2021, 143, 17015-17022.	6.6	15
205	Christoffel formula and geodesic motion in hyperspin manifolds. International Journal of Theoretical Physics, 1986, 25, 1209-1213.	0.5	14
206	Poor-solvent polyelectrolytes. Journal of Physics Condensed Matter, 2003, 15, S205-S211.	0.7	14
207	Screening of spherical colloids beyond mean field: A local density functional approach. Physical Review E, 2004, 69, 051401.	0.8	14
208	The influence of charged-induced variations in the local permittivity on the static and dynamic properties of polyelectrolyte solutions. Journal of Chemical Physics, 2015, 143, 243140.	1.2	14
209	Static polarizability effects on counterion distributions near charged dielectric surfaces: A coarse-grained Molecular Dynamics study employing the Drude model. European Physical Journal: Special Topics, 2016, 225, 1693-1705.	1.2	14
210	Modeling Gel Swelling Equilibrium in the Mean Field: From Explicit to Poisson-Boltzmann Models. Physical Review Letters, 2019, 122, 208002.	2.9	14
211	Ion pairing in model electrolytes: A study via three-particle correlation functions. Journal of Chemical Physics, 2003, 119, 4842-4856.	1.2	13
212	Modeling strategies for polyelectrolyte multilayers. European Physical Journal: Special Topics, 2009, 177, 129-148.	1.2	13
213	Properties of water in the interfacial region of a polyelectrolyte bilayer adsorbed onto a substrate studied by computer simulations. Physical Chemistry Chemical Physics, 2012, 14, 11425.	1.3	13
214	Electrophoretic mobility reversal of polyampholytes induced by strong electric fields or confinement. Journal of Chemical Physics, 2013, 138, 194905.	1.2	13
215	Layer-by-Layer Formation of Oligoelectrolyte Multilayers: A Combined Experimental and Computational Study. Soft Materials, 2014, 12, S14-S21.	0.8	13
216	Surface roughness stabilizes the clustering of self-propelled triangles. Journal of Chemical Physics, 2016, 145, 134904.	1.2	13

#	Article	IF	Citations
217	Three-body effects in triplets of capped gold nanocrystals. Molecular Physics, 2017, 115, 1031-1040.	0.8	13
218	Nanoparticle Translocation through Conical Nanopores: A Finite Element Study of Electrokinetic Transport. Macromolecular Theory and Simulations, 2017, 26, 1600051.	0.6	13
219	Modeling of weak polyelectrolyte hydrogels under compression â€“ Implications for water desalination. Desalination, 2021, 506, 114995.	4.0	13
220	Interactions of like-charged rods at low temperatures: Analytical theory vs. simulations. European Physical Journal E, 2008, 27, 21-9.	0.7	12
221	Structure factor of ferrofluids with chain aggregates: Theory and computer simulations. Journal of Magnetism and Magnetic Materials, 2011, 323, 1263-1268.	1.0	12
222	Effects of dielectric mismatch and chain flexibility on the translocation barriers of charged macromolecules through solid state nanopores. Soft Matter, 2012, 8, 9480.	1.2	12
223	Molecular Simulations of Hydrogels. , 2013, , 205-221.		12
224	Computing the Coulomb interaction in inhomogeneous dielectric media via a local electrostatics lattice algorithm. Physical Review E, 2014, 90, 063304.	0.8	12
225	Selective Trapping of DNA Using Glass Microcapillaries. Langmuir, 2016, 32, 8525-8532.	1.6	12
226	A computational model for bacterial run-and-tumble motion. Journal of Chemical Physics, 2019, 150, 174111.	1.2	12
227	On the Calculation of the Dielectric Properties of Liquid Ionic Systems. NATO Science for Peace and Security Series B: Physics and Biophysics, 2013, , 103-122.	0.2	12
228	Optimizing End-Labeled Free-Solution Electrophoresis by Increasing the Hydrodynamic Friction of the Drag Tag. Macromolecules, 2009, 42, 5352-5359.	2.2	11
229	The influence of motility on bacterial accumulation in a microporous channel. Soft Matter, 2021, 17, 893-902.	1.2	11
230	The pH-Dependent Swelling of Weak Polyelectrolyte Hydrogels Modeled at Different Levels of Resolution. Macromolecules, 2022, 55, 3176-3188.	2.2	11
231	Ground state structures in ferrofluid monolayers. Journal of Magnetism and Magnetic Materials, 2011, 323, 1298-1301.	1.0	10
232	The stretching force on a tethered polymer in pressure-driven flow. Journal of Chemical Physics, 2017, 147, 034902.	1.2	10
233	The hyperspin structure of unitary groups. Journal of Mathematical Physics, 1988, 29, 978-986.	0.5	9
234	Measuring the string susceptibility in 2D simplicial quantum gravity using the Regge approach. Nuclear Physics B, 1996, 477, 465-488.	0.9	9

#	Article	IF	Citations
235	Stability of Hydrophobically Modified Poly(p-phenylenesulfonate) Bundles As Observed by Molecular Dynamics Simulation. Macromolecules, 2007, 40, 1703-1707.	2.2	9
236	Multiscale Approaches and Perspectives to Modeling Aqueous Electrolytes and Polyelectrolytes. Topics in Current Chemistry, 2011, 307, 251-294.	4.0	9
237	Effective potentials between gold nano crystals â€“ functional dependence on temperature. Molecular Simulation, 2015, 41, 1153-1158.	0.9	9
238	A coarse-grained DNA model for the prediction of current signals in DNA translocation experiments. Journal of Chemical Physics, 2016, 145, 194106.	1.2	9
239	Conformation and Dynamics of Long-Chain End-Tethered Polymers in Microchannels. Polymers, 2019, 11, 488.	2.0	9
240	Cell Model Approaches for Predicting the Swelling and Mechanical Properties of Polyelectrolyte Gels. Macromolecules, 2019, 52, 9341-9353.	2.2	9
241	Elementary explanation of boundary shading in chaotic-attractor plots for the Feigenbaum map and the circle map. Physical Review A, 1986, 33, 2809-2812.	1.0	8
242	Hypergravitational field equations. Physical Review Letters, 1987, 59, 1265-1266.	2.9	8
243	High precision single-cluster Monte Carlo measurement of the critical exponents of the classical 3D Heisenberg model. Nuclear Physics, Section B, Proceedings Supplements, 1993, 30, 846-849.	0.5	8
244	Magnetic Flux Topology of 2D Point Dipoles. Computer Graphics Forum, 2012, 31, 955-964.	1.8	8
245	Monte Carlo study of asymmetric 2D XY model. Physica A: Statistical Mechanics and Its Applications, 1997, 246, 633-645.	1.2	7
246	Removal of spurious self-interactions in particleâ€“mesh methods. Computer Physics Communications, 2011, 182, 1919-1923.	3.0	7
247	Vapor-liquid coexistence of the Stockmayer fluid in nonuniform external fields. Physical Review E, 2013, 87, 052128.	0.8	7
248	Fixed versus random triangulations in 2D Regge calculus. Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics, 1997, 390, 59-63.	1.5	6
249	On the importance of hydrodynamic interactions in polyelectrolyte electrophoresis. Journal of Physics Condensed Matter, 2008, 20, 494217.	0.7	6
250	Particle-particle particle-mesh method for dipolar interactions: On error estimates and efficiency of schemes with analytical differentiation and mesh interlacing. Journal of Chemical Physics, 2011, 135, 184110.	1.2	6
251	Visual analysis for spaceâ€“time aggregation of biomolecular simulations. Faraday Discussions, 2014, 169, 167-178.	1.6	6
252	A dsDNA model optimized for electrokinetic applications. Soft Matter, 2017, 13, 3918-3926.	1.2	6

#	Article	IF	Citations
253	Can oppositely charged polyelectrolyte stars form a gel? A simulational study. Soft Matter, 2021, 17, 1574-1588.	1.2	6
254	Connections in Bergmann manifolds. International Journal of Theoretical Physics, 1990, 29, 23-36.	0.5	5
255	Modeling the current modulation of dsDNA in nanopores â€“ from mean-field to atomistic and back. European Physical Journal: Special Topics, 2019, 227, 1639-1655.	1.2	5
256	Atomistic simulation of PDADMAC/PSS oligoelectrolyte multilayers: overall comparison of tri- and tetra-layer systems. Soft Matter, 2019, 15, 9437-9451.	1.2	5
257	PDADMAC/PSS Oligoelectrolyte Multilayers: Internal Structure and Hydration Properties at Early Growth Stages from Atomistic Simulations. Molecules, 2020, 25, 1848.	1.7	5
258	Neutrino spectrum of Einstein universes. Journal of Mathematical Physics, 1988, 29, 2273-2279.	0.5	4
259	Measure dependence of 2D simplicial quantum gravity. Nuclear Physics, Section B, Proceedings Supplements, 1995, 42, 722-724.	0.5	4
260	The Ising transition in 2D simplicial quantum gravity â€” can Regge calculus be right?. Nuclear Physics, Section B, Proceedings Supplements, 1995, 42, 725-727.	0.5	4
261	Study of the structure factor anisotropy and long range correlations of ferrofluids in the dilute low-coupling regime. Journal of Magnetism and Magnetic Materials, 2011, 323, 1246-1253.	1.0	4
262	Accelerating the calculation of dipolar interactions in particle based simulations with open boundary conditions by means of the P2NFFT method. Journal of Computational Physics, 2019, 391, 243-258.	1.9	4
263	Developing coarse-grained models for agglomerate growth. European Physical Journal: Special Topics, 2019, 227, 1515-1527.	1.2	4
264	Modeling the current modulation of bundled DNA structures in nanopores. Journal of Chemical Physics, 2021, 154, 054901.	1.2	4
265	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
266	The Osmotic Behavior of Short Stiff Polyelectrolytes. Macromolecular Symposia, 2006, 245-246, 297-306.	0.4	3
267	Bidisperse monolayers: Theory and computer simulations. Physics Procedia, 2010, 9, 87-90.	1.2	3
268	Electric-field-induced stretching of surface-tethered polyelectrolytes in a microchannel. Physical Review E, 2017, 96, 032503.	0.8	3
269	Standard and Z2-Regge theory in two dimensions. Nuclear Physics, Section B, Proceedings Supplements, 1998, 63, 769-771.	0.5	2
270	SIMPLICIAL QUANTUM GRAVITY ON A RANDOMLY TRIANGULATED SPHERE. International Journal of Modern Physics A, 1999, 14, 3885-3903.	0.5	2

#	Article	IF	Citations
271	Z2-Regge versus standard Regge calculus in two dimensions. Physical Review D, 1999, 59, .	1.6	2
272	Polydispersity Influence upon Magnetic Properties of Aggregated Ferrofluids. Zeitschrift Fur Physikalische Chemie, 2006, 220, 105-115.	1.4	2
273	Simulating Charged Systems with ESPResSo. , 2006, , 193-221.		2
274	Novel Simulation Approaches for Polymeric and Soft Matter Systems. Macromolecular Theory and Simulations, 2011, 20, 444-445.	0.6	2
275	Microstructure of Bidisperse Ferrofluids in a Monolayer. Solid State Phenomena, 2012, 190, 625-628.	0.3	2
276	Preface: Special Topic on Coarse Graining of Macromolecules, Biopolymers, and Membranes. Journal of Chemical Physics, 2015, 143, 242901.	1.2	2
277	From the Atomistic to the Macromolecular Scale: Distinct Simulation Approaches for Polyelectrolyte Solutions. , 2018, , 1-15.		2
278	Particle methods in natural science and engineering. European Physical Journal: Special Topics, 2019, 227, 1493-1499.	1.2	2
279	Magnetic field controlled behavior of magnetic gels studied using particle-based simulations. ChemistrySelect, 2023, 8, 1465-1486.	0.7	2
280	A numerical investigation of analyte size effects in nanopore sensing systems. Journal of Chemical Physics, 2021, 155, 134902.	1.2	2
281	Computer Simulations of Charged Systems. , 2001, , 117-148.		2
282	New results on Î³str in 2D quantum gravity using Regge calculus. Nuclear Physics, Section B, Proceedings Supplements, 1996, 47, 621-624.	0.5	1
283	The Physics of Overcharging. , 2005, , 475-488.		1
284	Atomistic Simulation of Oligoelectrolyte Multilayers Growth. , 2016, , 215-228.		1
285	Relaxation of surface-tethered polymers under moderate confinement. Soft Matter, 2018, 14, 7926-7933.	1.2	1
286	Influence of weak groups on polyelectrolyte mobilities. Electrophoresis, 2019, 40, 799-809.	1.3	1
287	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
288	The control effort to steer self-propelled microswimmers depends on their morphology: comparing symmetric spherical versus asymmetric L -shaped particles. Royal Society Open Science, 2021, 8, 201839.	1.1	1

#	Article	IF	Citations
289	From the Atomistic to the Macromolecular Scale: Distinct Simulation Approaches for Polyelectrolyte Solutions. , 2020, , 1381-1395.		1
290	HIGH-PRECISION MONTE CARLO DETERMINATION OF Î±/Î½ IN THE 3D CLASSICAL HEISENBERG MODEL. International Journal of Modern Physics C, 1994, 05, 267-270.	0.8	0
291	Are defects important for 3D phase transitions?. Nuclear Physics, Section B, Proceedings Supplements, 1994, 34, 692-694.	0.5	0
292	Force Field Optimization for Ionic Liquids: FFOIL. , 2016, , 101-117.		0
293	Dynamics of field-driven population inversion in a confined colloidal mixture. Physical Review E, 2017, 95, 022605.	0.8	0