Christian Holm

List of Publications by Year
in descending order

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293 papers	12,729 citations	20817 60 h-index	38395 95 g-index
316 all docs	316 docs citations	316 times ranked	7378 citing authors

#	Article	IF	Citations
1	Magnetic field controlled behavior of magnetic gels studied using particle-based simulations. ChemistrySelect, 2023, 8, 1465-1486.	1.5	2
2	Order and information in the patterns of spinning magnetic micro-disks at the air-water interface. Science Advances, 2022, 8, eabk0685.	10.3	20
3	The pH-Dependent Swelling of Weak Polyelectrolyte Hydrogels Modeled at Different Levels of Resolution. Macromolecules, 2022, 55, 3176-3188.	4.8	11
4	A thermalized electrokinetics model including stochastic reactions suitable for multiscale simulations of reactionâ€“advectionâ€“diffusion systems. Journal of Computational Science, 2022, 63, 101770.	2.9	4
5	Can oppositely charged polyelectrolyte stars form a gel? A simulational study. Soft Matter, 2021, 17, 1574-1588.	2.7	6
6	The Presence of a Wall Enhances the Probability for Ringâ€€losing Metathesis: Insights from Classical Polymer Theory and Atomistic Simulations. Macromolecular Theory and Simulations, 2021, 30, 2000076.	1.4	1
7	Frequency-dependent magnetic susceptibility of magnetic nanoparticles in a polymer solution: a simulation study. Soft Matter, 2021, 17, 174-183.	2.7	17
8	An extensible lattice Boltzmann method for viscoelastic flows: complex and moving boundaries in Oldroyd-B fluids. European Physical Journal E, 2021, 44, 1.	1.6	23
9	Modeling the current modulation of bundled DNA structures in nanopores. Journal of Chemical Physics, 2021, 154, 054901.	3.0	4
10	Permeability Estimation of Regular Porous Structures: A Benchmark for Comparison of Methods. Transport in Porous Media, 2021, 138, 1-23.	2.6	18
11	Electrostatically Cross-Linked Reversible Gelsâ€”Effects of pH and Ionic Strength. Macromolecules, 2021, 54, 4769-4781.	4.8	15
12	Modeling of weak polyelectrolyte hydrogels under compression â€“ Implications for water desalination. Desalination, 2021, 506, 114995.	8.2	13
13	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.	2.4	1
14	Highly Efficient Active Colloids Driven by Galvanic Exchange Reactions. Journal of the American Chemical Society, 2021, 143, 17015-17022.	13.7	15
15	A numerical investigation of analyte size effects in nanopore sensing systems. Journal of Chemical Physics, 2021, 155, 134902.	3.0	2
16	The influence of motility on bacterial accumulation in a microporous channel. Soft Matter, 2021, 17, 893-902.	2.7	11
17	Ionic screening in bulk and under confinement. Journal of Chemical Physics, 2021, 155, 204501.	3.0	19
18	The Effect of Small Organic Cosolutes on Water Structure and Dynamics. Journal of Chemical & Engineering Data, 2020, 65, 1197-1210.	1.9	17

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19	DFT Accurate Interatomic Potential for Molten NaCl from Machine Learning. Journal of Physical Chemistry C, 2020, 124, 25760-25768.	3.1	39
20	How to speed up ion transport in nanopores. Nature Communications, 2020, 11, 6085.	12.8	57
21	Bulk ionic screening lengths from extremely large-scale molecular dynamics simulations. Chemical Communications, 2020, 56, 15635-15638.	4.1	30
22	Machine-learned interatomic potentials by active learning: amorphous and liquid hafnium dioxide. Npj Computational Materials, 2020, 6, .	8.7	100
23	PDADMAC/PSS Oligoelectrolyte Multilayers: Internal Structure and Hydration Properties at Early Growth Stages from Atomistic Simulations. Molecules, 2020, 25, 1848.	3.8	5
24	Grand-Reaction Method for Simulations of Ionization Equilibria Coupled to Ion Partitioning. Macromolecules, 2020, 53, 3007-3020.	4.8	44
25	From the Atomistic to the Macromolecular Scale: Distinct Simulation Approaches for Polyelectrolyte Solutions. , 2020, , 1381-1395.		1
26	Studying the field-controlled change of shape and elasticity of magnetic gels using particle-based simulations. Archive of Applied Mechanics, 2019, 89, 3-16.	2.2	23
27	A computational model for bacterial run-and-tumble motion. Journal of Chemical Physics, 2019, 150, 174111.	3.0	12
28	Hydrodynamic mobility reversal of squirmers near flat and curved surfaces. Soft Matter, 2019, 15, 5908-5920.	2.7	22
29	Simulations of ionization equilibria in weak polyelectrolyte solutions and gels. Soft Matter, 2019, 15, 1155-1185.	2.7	78
30	Influence of weak groups on polyelectrolyte mobilities. Electrophoresis, 2019, 40, 799-809.	2.4	1
31	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.	3.8	4
32	Modeling Gel Swelling Equilibrium in the Mean Field: From Explicit to Poisson-Boltzmann Models. Physical Review Letters, 2019, 122, 208002.	7.8	14
33	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.	2.6	5
34	A lattice Boltzmann model for squirmers. Journal of Chemical Physics, 2019, 150, 144110.	3.0	24
35	ESPResSo 4.0 â€“ an extensible software package for simulating soft matter systems. European Physical Journal: Special Topics, 2019, 227, 1789-1816.	2.6	127
36	Particle methods in natural science and engineering. European Physical Journal: Special Topics, 2019, 227, 1493-1499.	2.6	2

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37	Developing coarse-grained models for agglomerate growth. European Physical Journal: Special Topics, 2019, 227, 1515-1527.	2.6	4
38	Conformation and Dynamics of Long-Chain End-Tethered Polymers in Microchannels. Polymers, 2019, 11, 488.	4.5	9
39	Atomistic simulation of PDADMAC/PSS oligoelectrolyte multilayers: overall comparison of tri- and tetra-layer systems. Soft Matter, 2019, 15, 9437-9451.	2.7	5
40	Cell Model Approaches for Predicting the Swelling and Mechanical Properties of Polyelectrolyte Gels. Macromolecules, 2019, 52, 9341-9353.	4.8	9
41	Poly(sodium acrylate) hydrogels: synthesis of various network architectures, local molecular dynamics, salt partitioning, desalination and simulation. Soft Matter, 2019, 15, 9949-9964.	2.7	28
42	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.	3.1	22
43	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.	3.0	23
44	First-Principles Parametrization of Polarizable Coarse-Grained Force Fields for Ionic Liquids. Journal of Chemical Theory and Computation, 2018, 14, 1471-1486.	5.3	26
45	Polymer architecture of magnetic gels: a review. Journal of Physics Condensed Matter, 2018, 30, 063002.	1.8	73
46	Toward Understanding of Self-Electrophoretic Propulsion under Realistic Conditions: From Bulk Reactions to Confinement Effects. Accounts of Chemical Research, 2018, 51, 2998-3005.	15.6	19
47	Electrolyte solvents for high voltage lithium ion batteries: ion correlation and specific anion effects in adiponitrile. Physical Chemistry Chemical Physics, 2018, 20, 25701-25715.	2.8	41
48	Relaxation of surface-tethered polymers under moderate confinement. Soft Matter, 2018, 14, 7926-7933.	2.7	1
49	Specific ion effects for polyelectrolytes in aqueous and non-aqueous media: the importance of the ion solvation behavior. Soft Matter, 2018, 14, 6243-6255.	2.7	27
50	A polarizable MARTINI model for monovalent ions in aqueous solution. Journal of Chemical Physics, 2018, 149, 163319.	3.0	32
51	Computer Simulations of Static and Dynamical Properties of Weak Polyelectrolyte Nanogels in Salty Solutions. Gels, 2018, 4, 2.	4.5	17
52	From the Atomistic to the Macromolecular Scale: Distinct Simulation Approaches for Polyelectrolyte Solutions. , 2018, , 1-15.		2
53	Charge Me Slowly, I Am in a Hurry: Optimizing Chargeâ€“Discharge Cycles in Nanoporous Supercapacitors. ACS Nano, 2018, 12, 9733-9741.	14.6	80
54	Microfluidic pumping by micromolar salt concentrations. Soft Matter, 2017, 13, 1505-1518.	2.7	46

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55	Wangâ€“Landau Reaction Ensemble Method: Simulation of Weak Polyelectrolytes and General Acidâ€“Base Reactions. Journal of Chemical Theory and Computation, 2017, 13, 852-862.	5.3	17
56	A refined polarizable water model for the coarse-grained MARTINI force field with long-range electrostatic interactions. Journal of Chemical Physics, 2017, 146, 054501.	3.0	69
57	A self-consistent mean-field model for polyelectrolyte gels. Soft Matter, 2017, 13, 3264-3274.	2.7	34
58	Simulation of weak polyelectrolytes: a comparison between the constant pH and the reaction ensemble method. European Physical Journal: Special Topics, 2017, 226, 725-736.	2.6	40
59	A dsDNA model optimized for electrokinetic applications. Soft Matter, 2017, 13, 3918-3926.	2.7	6
60	Three-body effects in triplets of capped gold nanocrystals. Molecular Physics, 2017, 115, 1031-1040.	1.7	13
61	On the efficiency of a hydrogel-based desalination cycle. Desalination, 2017, 414, 28-34.	8.2	33
62	Ionic screening and dissociation are crucial for understanding chemical self-propulsion in polar solvents. Soft Matter, 2017, 13, 1200-1222.	2.7	95
63	Electric-field-induced stretching of surface-tethered polyelectrolytes in a microchannel. Physical Review E, 2017, 96, 032503.	2.1	3
64	The effect of finite pore length on ion structure and charging. Journal of Chemical Physics, 2017, 147, 104708.	3.0	29
65	The stretching force on a tethered polymer in pressure-driven flow. Journal of Chemical Physics, 2017, 147, 034902.	3.0	10
66	Nanoparticle Translocation through Conical Nanopores: A Finite Element Study of Electrokinetic Transport. Macromolecular Theory and Simulations, 2017, 26, 1600051.	1.4	13
67	Stretching of surface-tethered polymers in pressure-driven flow under confinement. Soft Matter, 2017, 13, 6189-6196.	2.7	15
68	A coarse-grained polarizable force field for the ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate. Journal of Physics Condensed Matter, 2017, 29, 504004.	1.8	16
69	Dynamics of field-driven population inversion in a confined colloidal mixture. Physical Review E, 2017, 95, 022605.	2.1	0
70	Properties of Apolar Solutes in Alkyl Imidazoliumâ€Based Ionic Liquids: The Importance of Local Interactions. ChemPhysChem, 2016, 17, 387-394.	2.1	28
71	Reducing spurious flow in simulations of electrokinetic phenomena. Journal of Chemical Physics, 2016, 145, 044901.	3.0	21
72	Surface roughness stabilizes the clustering of self-propelled triangles. Journal of Chemical Physics, 2016, 145, 134904.	3.0	13

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73	Lattice-Boltzmann hydrodynamics of anisotropic active matter. Journal of Chemical Physics, 2016, 144, 134106.	3.0	40
74	A coarse-grained DNA model for the prediction of current signals in DNA translocation experiments. Journal of Chemical Physics, 2016, 145, 194106.	3.0	9
75	Moving charged particles in lattice Boltzmann-based electrokinetics. Journal of Chemical Physics, 2016, 145, 214102.	3.0	23
76	Understanding the onset of oscillatory swimming in microchannels. Soft Matter, 2016, 12, 4704-4708.	2.7	25
77	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.	4.6	72
78	Selective Trapping of DNA Using Glass Microcapillaries. Langmuir, 2016, 32, 8525-8532.	3.5	12
79	Preferential solvation and ion association properties in aqueous dimethyl sulfoxide solutions. Physical Chemistry Chemical Physics, 2016, 18, 31312-31322.	2.8	30
80	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.	2.6	14
81	The efficiency of self-phoretic propulsion mechanisms with surface reaction heterogeneity. Journal of Chemical Physics, 2016, 144, 204902.	3.0	21
82	Atomistic Simulation of Oligoelectrolyte Multilayers Growth. , 2016, , 215-228.		1
83	Force Field Optimization for Ionic Liquids: FFOIL. , 2016, , 101-117.		0
84	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.	2.8	61
85	Buckling of paramagnetic chains in soft gels. Soft Matter, 2016, 12, 228-237.	2.7	68
86	Importance of Varying Permittivity on the Conductivity of Polyelectrolyte Solutions. Physical Review Letters, 2015, 115, 118301.	7.8	33
87	Ferrogels cross-linked by magnetic particles: Field-driven deformation and elasticity studied using computer simulations. Journal of Chemical Physics, 2015, 143, 154901.	3.0	40
88	Preface: Special Topic on Coarse Graining of Macromolecules, Biopolymers, and Membranes. Journal of Chemical Physics, 2015, 143, 242901.	3.0	2
89	The raspberry model for hydrodynamic interactions revisited. I. Periodic arrays of spheres and dumbbells. Journal of Chemical Physics, 2015, 143, 084107.	3.0	40
90	Coarse-grained simulations of polyelectrolyte complexes: MARTINI models for poly(styrene sulfonate) and poly(diallyldimethylammonium). Journal of Chemical Physics, 2015, 143, 243151.	3.0	69

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91	The Raspberry model for hydrodynamic interactions revisited. II. The effect of confinement. Journal of Chemical Physics, 2015, 143, 084108.	3.0	26
92	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.	3.0	14
93	Effective potentials between gold nano crystals â€“ functional dependence on temperature. Molecular Simulation, 2015, 41, 1153-1158.	2.0	9
94	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.	2.8	40
95	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.	4.8	20
96	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.	2.3	48
97	Diffusiophoretic Self-Propulsion for Partially Catalytic Spherical Colloids. IEEE Transactions on Nanobioscience, 2015, 14, 272-288.	3.3	29
98	Coarse-grained molecular dynamics simulation of small ferrogel objects. Journal of Magnetism and Magnetic Materials, 2015, 383, 277-280.	2.3	21
99	Towards a scale-bridging description of ferrogels and magnetic elastomers. Journal of Physics Condensed Matter, 2015, 27, 325105.	1.8	25
100	Electrode Models for Ionic Liquid-Based Capacitors. Journal of Physical Chemistry C, 2015, 119, 22445-22451.	3.1	54
101	Peptides in the presence of aqueous ionic liquids: tunable co-solutes as denaturants or protectants?. Physical Chemistry Chemical Physics, 2015, 17, 26049-26053.	2.8	48
102	Modeling of Polyelectrolyte Gels in Equilibrium with Salt Solutions. Macromolecules, 2015, 48, 7698-7708.	4.8	72
103	Properties of the polarizable MARTINI water model: A comparative study for aqueous electrolyte solutions. Journal of Molecular Liquids, 2015, 212, 103-110.	4.9	25
104	Computing the Coulomb interaction in inhomogeneous dielectric media via a local electrostatics lattice algorithm. Physical Review E, 2014, 90, 063304.	2.1	12
105	Lattice-Boltzmann simulations of the electrophoretic stretching of polyelectrolytes: The importance of hydrodynamic interactions. Journal of Chemical Physics, 2014, 140, 164904.	3.0	16
106	Mobility Reversal of Polyelectrolyte-Grafted Colloids in Monovalent Salt Solutions. Physical Review Letters, 2014, 113, 238301.	7.8	29
107	Origin of Current Blockades in Nanopore Translocation Experiments. Physical Review Letters, 2014, 112, 018101.	7.8	51
108	Communication: Kinetic and pairing contributions in the dielectric spectra of electrolyte solutions. Journal of Chemical Physics, 2014, 140, 211101.	3.0	25

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109	Simulation of electric double layers around charged colloids in aqueous solution of variable permittivity. Journal of Chemical Physics, 2014, 141, 064902.	3.0	29
110	The solvation and ion condensation properties for sulfonated polyelectrolytes in different solventsâ€"a computational study. New Journal of Physics, 2014, 16, 025001.	2.9	40
111	Generic force fields for ionic liquids. Journal of Molecular Liquids, 2014, 192, 32-37.	4.9	32
112	Visual analysis for spaceâ€"time aggregation of biomolecular simulations. Faraday Discussions, 2014, 169, 167-178.	3.2	6
113	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.	2.6	32
114	Layer-by-Layer Formation of Oligoelectrolyte Multilayers: A Combined Experimental and Computational Study. Soft Materials, 2014, 12, S14-S21.	1.7	13
115	Computing the Electrophoretic Mobility of Large Spherical Colloids by Combining Explicit Ion Simulations with the Standard Electrokinetic Model. Langmuir, 2014, 30, 1758-1767.	3.5	18
116	Coarse-grained simulations of an ionic liquid-based capacitor: I. Density, ion size, and valency effects. Journal of Physics Condensed Matter, 2014, 26, 284108.	1.8	25
117	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.	1.8	17
118	Dynamics in Stimuli-Responsive Poly(N-isopropylacrylamide) Hydrogel Layers As Revealed by Fluorescence Correlation Spectroscopy. Macromolecules, 2014, 47, 5303-5312.	4.8	31
119	ESPResSo 3.1: Molecular Dynamics Software for Coarse-Grained Models. Lecture Notes in Computational Science and Engineering, 2013, , 1-23.	0.3	118
120	Complex Tracer Diffusion Dynamics in Polymer Solutions. Physical Review Letters, 2013, 111, 088301.	7.8	50
121	Refining classical force fields for ionic liquids: theory and application to [MMIM][Cl]. Physical Chemistry Chemical Physics, 2013, 15, 2037-2049.	2.8	23
122	Cluster formation in systems of shifted-dipole particles. Soft Matter, 2013, 9, 3535.	2.7	32
123	Phase diagram for a single flexible Stockmayer polymer at zero field. Soft Matter, 2013, 9, 7185.	2.7	26
124	Comparison of scalable fast methods for long-range interactions. Physical Review E, 2013, 88, 063308.	2.1	72
125	Vapor-liquid coexistence of the Stockmayer fluid in nonuniform external fields. Physical Review E, 2013, 87, 052128.	2.1	7
126	Electrophoretic mobility and charge inversion of a colloidal particle studied by single-colloid electrophoresis and molecular dynamics simulations. Physical Review E, 2013, 87, 022302.	2.1	64

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127	Effects of the dipolar interaction on the equilibrium morphologies of a single supramolecular magnetic filament in bulk. Journal of Chemical Physics, 2013, 139, 044904.	3.0	28
128	Electrophoretic mobility reversal of polyampholytes induced by strong electric fields or confinement. Journal of Chemical Physics, 2013, 138, 194905.	3.0	13
129	Efficient Algorithms for Electrostatic Interactions Including Dielectric Contrasts. Entropy, 2013, 15, 4569-4588.	2.2	41
130	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.	3.0	23
131	Molecular Simulations of Hydrogels. , 2013, , 205-221.		12
132	Tracer diffusion in a crowded cylindrical channel. Physical Review E, 2013, 87, 062709.	2.1	21
133	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.	0.3	12
134	Microstructure of Bidisperse Ferrofluids in a Monolayer. Solid State Phenomena, 2012, 190, 625-628.	0.3	2
135	Deformation mechanisms in 2D magnetic gels studied by computer simulations. Soft Matter, 2012, 8, 9923.	2.7	87
136	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.	2.8	13
137	How to Convert SPME to P3M: Influence Functions and Error Estimates. Journal of Chemical Theory and Computation, 2012, 8, 936-947.	5.3	21
138	Ionic liquids studied across different scales: A computational perspective. Faraday Discussions, 2012, 154, 111-132.	3.2	99
139	Effects of dielectric mismatch and chain flexibility on the translocation barriers of charged macromolecules through solid state nanopores. Soft Matter, 2012, 8, 9480.	2.7	12
140	Force Fields for Studying the Structure and Dynamics of Ionic Liquids: A Critical Review of Recent Developments. ChemPhysChem, 2012, 13, 1625-1637.	2.1	239
141	Magnetic Flux Topology of 2D Point Dipoles. Computer Graphics Forum, 2012, 31, 955-964.	3.0	8
142	Semiflexible magnetic filaments near attractive flat surfaces: a Langevin dynamics study. Soft Matter, 2011, 7, 1809-1818.	2.7	16
143	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.	2.8	21
144	Ferrofluids with shifted dipoles: ground state structures. Soft Matter, 2011, 7, 5217.	2.7	46

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145	Influence of Charged Polymer Coatings on Electro-Osmotic Flow: Molecular Dynamics Simulations. Macromolecules, 2011, 44, 9455-9463.	4.8	30
146	Atomistic Study of Surface Effects on Polyelectrolyte Adsorption: Case Study of a Poly(styrenesulfonate) Monolayer. Macromolecules, 2011, 44, 1707-1718.	4.8	33
147	Locality and Fluctuations: Trends in Imidazolium-Based Ionic Liquids and Beyond. Journal of Chemical Theory and Computation, 2011, 7, 3040-3044.	5.3	93
148	Simulational study of anomalous tracer diffusion in hydrogels. Colloid and Polymer Science, 2011, 289, 523-534.	2.1	31
149	Removal of spurious self-interactions in particleâ€“mesh methods. Computer Physics Communications, 2011, 182, 1919-1923.	7.5	7
150	Hydrogels in Poor Solvents: A Molecular Dynamics Study. Macromolecular Theory and Simulations, 2011, 20, 721-734.	1.4	44
151	Novel Simulation Approaches for Polymeric and Soft Matter Systems. Macromolecular Theory and Simulations, 2011, 20, 444-445.	1.4	2
152	Applying to DNA translocation: Effect of dielectric boundaries. Computer Physics Communications, 2011, 182, 33-35.	7.5	19
153	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.	2.3	4
154	Structure factor of ferrofluids with chain aggregates: Theory and computer simulations. Journal of Magnetism and Magnetic Materials, 2011, 323, 1263-1268.	2.3	12
155	Magnetic particles with shifted dipoles. Journal of Magnetism and Magnetic Materials, 2011, 323, 1269-1272.	2.3	22
156	Ground state structures in ferrofluid monolayers. Journal of Magnetism and Magnetic Materials, 2011, 323, 1298-1301.	2.3	10
157	Multiscale Approaches and Perspectives to Modeling Aqueous Electrolytes and Polyelectrolytes. Topics in Current Chemistry, 2011, 307, 251-294.	4.0	9
158	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.	3.0	38
159	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.	3.0	6
160	Behavior of bulky ferrofluids in the diluted low-coupling regime: Theory and simulation. Physical Review E, 2010, 81, 011501.	2.1	30
161	Bidisperse monolayers: Theory and computer simulations. Physics Procedia, 2010, 9, 87-90.	1.2	3
162	Towards multiscale modeling of ionic liquids: From electronic structure to bulk properties. Journal of Molecular Liquids, 2010, 152, 2-8.	4.9	50

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163	An iterative, fast, linear-scaling method for computing induced charges on arbitrary dielectric boundaries. Journal of Chemical Physics, 2010, 132, 154112.	3.0	76
164	Optimizing working parameters of the smooth particle mesh Ewald algorithm in terms of accuracy and efficiency. Journal of Chemical Physics, 2010, 133, 034117.	3.0	108
165	Interlaced P3M algorithm with analytical and ik-differentiation. Journal of Chemical Physics, 2010, 132, 234103.	3.0	26
166	Implicit Method for Simulating Electrohydrodynamics of Polyelectrolytes. Physical Review Letters, 2010, 105, 148301.	7.8	22
167	Equilibrium polyelectrolyte bundles with different multivalent counterion concentrations. Physical Review E, 2010, 82, 031901.	2.1	22
168	Poly(styrenesulfonate)â^'Poly(diallyldimethylammonium) Mixtures: Toward the Understanding of Polyelectrolyte Complexes and Multilayers via Atomistic Simulations. Macromolecules, 2010, 43, 7828-7838.	4.8	45
169	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.	2.6	113
170	Mesoscale modelling of polyelectrolyteelectrophoresis. Faraday Discussions, 2010, 144, 57-70.	3.2	28
171	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.	2.8	38
172	Ground state structures in ferrofluid monolayers. Physical Review E, 2009, 80, 031404.	2.1	64
173	Comparison of a hydrogel model to the Poissonâ€“Boltzmann cell model. Journal of Chemical Physics, 2009, 131, 094903.	3.0	69
174	Ensemble inequivalence in single-molecule experiments. Physical Review E, 2009, 79, 051118.	2.1	26
175	Modeling the separation of macromolecules: A review of current computer simulation methods. Electrophoresis, 2009, 30, 792-818.	2.4	126
176	Modeling strategies for polyelectrolyte multilayers. European Physical Journal: Special Topics, 2009, 177, 129-148.	2.6	13
177	Optimizing End-Labeled Free-Solution Electrophoresis by Increasing the Hydrodynamic Friction of the Drag Tag. Macromolecules, 2009, 42, 5352-5359.	4.8	11
178	Understanding polyelectrolyte multilayers: an open challenge for simulations. Soft Matter, 2009, 5, 4412.	2.7	54
179	Polyelectrolytes in electric fields: measuring the dynamical effective charge and effective friction. Soft Matter, 2009, 5, 2079.	2.7	58
180	How to analyse the structure factor in ferrofluids with strong magnetic interactions: a combined analytic and simulation approach. Molecular Physics, 2009, 107, 571-590.	1.7	29

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181	Mesoscopic simulations of the counterion-induced electro-osmotic flow: A comparative study. Journal of Chemical Physics, 2009, 130, 244702.	3.0	48
182	Simulation of charge reversal in salty environments: Giant overcharging?. European Physical Journal E, 2008, 26, 191-195.	1.6	41
183	Interactions of like-charged rods at low temperatures: Analytical theory vs. simulations. European Physical Journal E, 2008, 27, 21-9.	1.6	12
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