Christian Holm

List of Publications by Year in Descending Order

293 papers	10,872 citations	55 h-index	89 g-index
316 ext. papers	11,726 ext. citations	3.7 avg, IF	6.59 L-index

#	Paper	IF	Citations
293	Order and information in the patterns of spinning magnetic micro-disks at the air-water interface.. *Science Advances*, **2022**, 8, eabk0685	14.3	5
292	Ionic screening in bulk and under confinement. *Journal of Chemical Physics*, **2021**, 155, 204501	3.9	2
291	Permeability Estimation of Regular Porous Structures: A Benchmark for Comparison of Methods. *Transport in Porous Media*, **2021**, 138, 1-23	3.1	2
290	Electrostatically Cross-Linked Reversible Gels Effects of pH and Ionic Strength. *Macromolecules*, **2021**, 54, 4769-4781	5.5	1
289	Modeling of weak polyelectrolyte hydrogels under compression Implications for water desalination. *Desalination*, **2021**, 506, 114995	10.3	3
288	Can oppositely charged polyelectrolyte stars form a gel? A simulational study. *Soft Matter*, **2021**, 17, 1574-1588	3.6	1
287	The Presence of a Wall Enhances the Probability for Ring-Closing Metathesis: Insights from Classical Polymer Theory and Atomistic Simulations. *Macromolecular Theory and Simulations*, **2021**, 30, 2000076	1.5	
286	Frequency-dependent magnetic susceptibility of magnetic nanoparticles in a polymer solution: a simulation study. *Soft Matter*, **2021**, 17, 174-183	3.6	8
285	An extensible lattice Boltzmann method for viscoelastic flows: complex and moving boundaries in Oldroyd-B fluids. *European Physical Journal E*, **2021**, 44, 1	1.5	6
284	Modeling the current modulation of bundled DNA structures in nanopores. *Journal of Chemical Physics*, **2021**, 154, 054901	3.9	3
283	The control effort to steer self-propelled microswimmers depends on their morphology: comparing symmetric spherical versus asymmetric -shaped particles. *Royal Society Open Science*, **2021**, 8, 201839	3.3	
282	Highly Efficient Active Colloids Driven by Galvanic Exchange Reactions. *Journal of the American Chemical Society*, **2021**, 143, 17015-17022	16.4	4
281	A numerical investigation of analyte size effects in nanopore sensing systems. *Journal of Chemical Physics*, **2021**, 155, 134902	3.9	0
280	The influence of motility on bacterial accumulation in a microporous channel. *Soft Matter*, **2021**, 17, 893-902	3.6	0
279	PDADMAC/PSS Oligoelectrolyte Multilayers: Internal Structure and Hydration Properties at Early Growth Stages from Atomistic Simulations. *Molecules*, **2020**, 25,	4.8	1
278	From the Atomistic to the Macromolecular Scale: Distinct Simulation Approaches for Polyelectrolyte Solutions **2020**, 1381-1395		
277	DFT Accurate Interatomic Potential for Molten NaCl from Machine Learning. *Journal of Physical Chemistry C*, **2020**, 124, 25760-25768	3.8	16

276	How to speed up ion transport in nanopores. *Nature Communications*, **2020**, 11, 6085	17.4	22
275	Bulk ionic screening lengths from extremely large-scale molecular dynamics simulations. *Chemical Communications*, **2020**, 56, 15635-15638	5.8	14
274	Machine-learned interatomic potentials by active learning: amorphous and liquid hafnium dioxide. *Npj Computational Materials*, **2020**, 6,	10.9	34
273	The Effect of Small Organic Cosolutes on Water Structure and Dynamics. *Journal of Chemical & Engineering Data*, **2020**, 65, 1197-1210	2.8	14
272	Grand-Reaction Method for Simulations of Ionization Equilibria Coupled to Ion Partitioning. *Macromolecules*, **2020**, 53, 3007-3020	5.5	17
271	Simulations of ionization equilibria in weak polyelectrolyte solutions and gels. *Soft Matter*, **2019**, 15, 1155-1185	3.6	41
270	Influence of weak groups on polyelectrolyte mobilities. *Electrophoresis*, **2019**, 40, 799-809	3.6	1
269	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	4.1	1
268	Modeling Gel Swelling Equilibrium in the Mean Field: From Explicit to Poisson-Boltzmann Models. *Physical Review Letters*, **2019**, 122, 208002	7.4	9
267	Modeling the current modulation of dsDNA in nanopores from mean-field to atomistic and back. *European Physical Journal: Special Topics*, **2019**, 227, 1639-1655	2.3	2
266	A lattice Boltzmann model for squirmers. *Journal of Chemical Physics*, **2019**, 150, 144110	3.9	15
265	ESPResSo 4.0 an extensible software package for simulating soft matter systems. *European Physical Journal: Special Topics*, **2019**, 227, 1789-1816	2.3	62
264	Developing coarse-grained models for agglomerate growth. *European Physical Journal: Special Topics*, **2019**, 227, 1515-1527	2.3	3
263	Conformation and Dynamics of Long-Chain End-Tethered Polymers in Microchannels. *Polymers*, **2019**, 11,	4.5	5
262	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	16
261	A computational model for bacterial run-and-tumble motion. *Journal of Chemical Physics*, **2019**, 150, 174111	3.9	5
260	Hydrodynamic mobility reversal of squirmers near flat and curved surfaces. *Soft Matter*, **2019**, 15, 5908-5920	3.6	15
259	Atomistic simulation of PDADMAC/PSS oligoelectrolyte multilayers: overall comparison of tri- and tetra-layer systems. *Soft Matter*, **2019**, 15, 9437-9451	3.6	4

258	Cell Model Approaches for Predicting the Swelling and Mechanical Properties of Polyelectrolyte Gels. *Macromolecules*, **2019**, 52, 9341-9353	5.5	4
257	Poly(sodium acrylate) hydrogels: synthesis of various network architectures, local molecular dynamics, salt partitioning, desalination and simulation. *Soft Matter*, **2019**, 15, 9949-9964	3.6	17
256	Influence of Cosolutes on Chemical Equilibrium: a KirkwoodBuff Theory for Ion Pair AssociationDissociation Processes in Ternary Electrolyte Solutions. *Journal of Physical Chemistry C*, **2018**, 122, 10293-10302	3.8	20
255	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	3.9	19
254	First-Principles Parametrization of Polarizable Coarse-Grained Force Fields for Ionic Liquids. *Journal of Chemical Theory and Computation*, **2018**, 14, 1471-1486	6.4	19
253	Polymer architecture of magnetic gels: a review. *Journal of Physics Condensed Matter*, **2018**, 30, 063002	1.8	51
252	A polarizable MARTINI model for monovalent ions in aqueous solution. *Journal of Chemical Physics*, **2018**, 149, 163319	3.9	17
251	From the Atomistic to the Macromolecular Scale: Distinct Simulation Approaches for Polyelectrolyte Solutions **2018**, 1-15		1
250	Charge Me Slowly, I Am in a Hurry: Optimizing Charge-Discharge Cycles in Nanoporous Supercapacitors. *ACS Nano*, **2018**, 12, 9733-9741	16.7	54
249	Toward Understanding of Self-Electrophoretic Propulsion under Realistic Conditions: From Bulk Reactions to Confinement Effects. *Accounts of Chemical Research*, **2018**, 51, 2998-3005	24.3	9
248	Electrolyte solvents for high voltage lithium ion batteries: ion correlation and specific anion effects in adiponitrile. *Physical Chemistry Chemical Physics*, **2018**, 20, 25701-25715	3.6	26
247	Relaxation of surface-tethered polymers under moderate confinement. *Soft Matter*, **2018**, 14, 7926-7933	3.6	1
246	Specific ion effects for polyelectrolytes in aqueous and non-aqueous media: the importance of the ion solvation behavior. *Soft Matter*, **2018**, 14, 6243-6255	3.6	18
245	Microfluidic pumping by micromolar salt concentrations. *Soft Matter*, **2017**, 13, 1505-1518	3.6	36
244	Wang-Landau Reaction Ensemble Method: Simulation of Weak Polyelectrolytes and General Acid-Base Reactions. *Journal of Chemical Theory and Computation*, **2017**, 13, 852-862	6.4	14
243	A refined polarizable water model for the coarse-grained MARTINI force field with long-range electrostatic interactions. *Journal of Chemical Physics*, **2017**, 146, 054501	3.9	47
242	A self-consistent mean-field model for polyelectrolyte gels. *Soft Matter*, **2017**, 13, 3264-3274	3.6	27
241	Simulation of weak polyelectrolytes: a comparison between the constant pH and the reaction ensemble method. *European Physical Journal: Special Topics*, **2017**, 226, 725-736	2.3	30

240	A dsDNA model optimized for electrokinetic applications. *Soft Matter*, **2017**, 13, 3918-3926	3.6	5
239	Three-body effects in triplets of capped gold nanocrystals. *Molecular Physics*, **2017**, 115, 1031-1040	1.7	9
238	On the efficiency of a hydrogel-based desalination cycle. *Desalination*, **2017**, 414, 28-34	10.3	19
237	Ionic screening and dissociation are crucial for understanding chemical self-propulsion in polar solvents. *Soft Matter*, **2017**, 13, 1200-1222	3.6	74
236	Electric-field-induced stretching of surface-tethered polyelectrolytes in a microchannel. *Physical Review E*, **2017**, 96, 032503	2.4	2
235	Computer Simulations of Static and Dynamical Properties of Weak Polyelectrolyte Nanogels in Salty Solutions. *Gels*, **2017**, 4,	4.2	14
234	The effect of finite pore length on ion structure and charging. *Journal of Chemical Physics*, **2017**, 147, 104708	3.9	24
233	The stretching force on a tethered polymer in pressure-driven flow. *Journal of Chemical Physics*, **2017**, 147, 034902	3.9	9
232	Nanoparticle Translocation through Conical Nanopores: A Finite Element Study of Electrokinetic Transport. *Macromolecular Theory and Simulations*, **2017**, 26, 1600051	1.5	9
231	Stretching of surface-tethered polymers in pressure-driven flow under confinement. *Soft Matter*, **2017**, 13, 6189-6196	3.6	11
230	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	14
229	Dynamics of field-driven population inversion in a confined colloidal mixture. *Physical Review E*, **2017**, 95, 022605	2.4	
228	Buckling of paramagnetic chains in soft gels. *Soft Matter*, **2016**, 12, 228-37	3.6	59
227	Preferential solvation and ion association properties in aqueous dimethyl sulfoxide solutions. *Physical Chemistry Chemical Physics*, **2016**, 18, 31312-31322	3.6	22
226	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	2.3	10
225	The efficiency of self-phoretic propulsion mechanisms with surface reaction heterogeneity. *Journal of Chemical Physics*, **2016**, 144, 204902	3.9	19
224	Correction to Modeling of Polyelectrolyte Gels in Equilibrium with Salt Solutions. *Macromolecules*, **2016**, 49, 2409-2409	5.5	2
223	Atomistic Simulation of Oligoelectrolyte Multilayers Growth **2016**, 215-228		1

222	Force Field Optimization for Ionic Liquids: FFOIL **2016**, 101-117		
221	Concentration dependent effects of urea binding to poly(N-isopropylacrylamide) brushes: a combined experimental and numerical study. *Physical Chemistry Chemical Physics*, **2016**, 18, 5324-35	3.6	54
220	Properties of Apolar Solutes in Alkyl Imidazolium-Based Ionic Liquids: The Importance of Local Interactions. *ChemPhysChem*, **2016**, 17, 387-94	3.2	26
219	Reducing spurious flow in simulations of electrokinetic phenomena. *Journal of Chemical Physics*, **2016**, 145, 044901	3.9	19
218	Surface roughness stabilizes the clustering of self-propelled triangles. *Journal of Chemical Physics*, **2016**, 145, 134904	3.9	11
217	Lattice-Boltzmann hydrodynamics of anisotropic active matter. *Journal of Chemical Physics*, **2016**, 144, 134106	3.9	29
216	A coarse-grained DNA model for the prediction of current signals in DNA translocation experiments. *Journal of Chemical Physics*, **2016**, 145, 194106	3.9	8
215	Moving charged particles in lattice Boltzmann-based electrokinetics. *Journal of Chemical Physics*, **2016**, 145, 214102	3.9	17
214	Understanding the onset of oscillatory swimming in microchannels. *Soft Matter*, **2016**, 12, 4704-8	3.6	24
213	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	6.4	62
212	Selective Trapping of DNA Using Glass Microcapillaries. *Langmuir*, **2016**, 32, 8525-32	4	11
211	Ferrogels cross-linked by magnetic nanoparticles—Deformation mechanisms in two and three dimensions studied by means of computer simulations. *Journal of Magnetism and Magnetic Materials*, **2015**, 383, 262-266	2.8	38
210	Diffusiophoretic self-propulsion for partially catalytic spherical colloids. *IEEE Transactions on Nanobioscience*, **2015**, 14, 272-88	3.4	27
209	Coarse-grained molecular dynamics simulation of small ferrogel objects. *Journal of Magnetism and Magnetic Materials*, **2015**, 383, 277-280	2.8	20
208	Towards a scale-bridging description of ferrogels and magnetic elastomers. *Journal of Physics Condensed Matter*, **2015**, 27, 325105	1.8	21
207	Electrode Models for Ionic Liquid-Based Capacitors. *Journal of Physical Chemistry C*, **2015**, 119, 22445-22451	4.5	41
206	Peptides in the presence of aqueous ionic liquids: tunable co-solutes as denaturants or protectants?. *Physical Chemistry Chemical Physics*, **2015**, 17, 26049-53	3.6	44
205	Modeling of Polyelectrolyte Gels in Equilibrium with Salt Solutions. *Macromolecules*, **2015**, 48, 7698-7708	5.5	57

204	Properties of the polarizable MARTINI water model: A comparative study for aqueous electrolyte solutions. *Journal of Molecular Liquids*, **2015**, 212, 103-110	6	23
203	Importance of varying permittivity on the conductivity of polyelectrolyte solutions. *Physical Review Letters*, **2015**, 115, 118301	7.4	28
202	Ferrogels cross-linked by magnetic particles: Field-driven deformation and elasticity studied using computer simulations. *Journal of Chemical Physics*, **2015**, 143, 154901	3.9	30
201	Preface: Special Topic on Coarse Graining of Macromolecules, Biopolymers, and Membranes. *Journal of Chemical Physics*, **2015**, 143, 242901	3.9	2
200	The raspberry model for hydrodynamic interactions revisited. I. Periodic arrays of spheres and dumbbells. *Journal of Chemical Physics*, **2015**, 143, 084107	3.9	30
199	Coarse-grained simulations of polyelectrolyte complexes: MARTINI models for poly(styrene sulfonate) and poly(diallyldimethylammonium). *Journal of Chemical Physics*, **2015**, 143, 243151	3.9	55
198	The Raspberry model for hydrodynamic interactions revisited. II. The effect of confinement. *Journal of Chemical Physics*, **2015**, 143, 084108	3.9	22
197	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	3.9	14
196	Effective potentials between gold nano crystals Functional dependence on temperature. *Molecular Simulation*, **2015**, 41, 1153-1158	2	9
195	Solvent effects of 1-ethyl-3-methylimidazolium acetate: solvation and dynamic behavior of polar and apolar solutes. *Physical Chemistry Chemical Physics*, **2015**, 17, 8480-90	3.6	36
194	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	5.5	19
193	Generic force fields for ionic liquids. *Journal of Molecular Liquids*, **2014**, 192, 32-37	6	30
192	Visual analysis for space-time aggregation of biomolecular simulations. *Faraday Discussions*, **2014**, 169, 167-78	3.6	5
191	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, 11613-21	3.4	31
190	Layer-by-Layer Formation of Oligoelectrolyte Multilayers: A Combined Experimental and Computational Study. *Soft Materials*, **2014**, 12, S14-S21	1.7	11
189	Computing the electrophoretic mobility of large spherical colloids by combining explicit ion simulations with the standard electrokinetic model. *Langmuir*, **2014**, 30, 1758-67	4	16
188	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	21
187	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	15

186	Dynamics in Stimuli-Responsive Poly(N-isopropylacrylamide) Hydrogel Layers As Revealed by Fluorescence Correlation Spectroscopy. *Macromolecules*, **2014**, 47, 5303-5312	5.5	24
185	Computing the Coulomb interaction in inhomogeneous dielectric media via a local electrostatics lattice algorithm. *Physical Review E*, **2014**, 90, 063304	2.4	11
184	Lattice-Boltzmann simulations of the electrophoretic stretching of polyelectrolytes: the importance of hydrodynamic interactions. *Journal of Chemical Physics*, **2014**, 140, 164904	3.9	15
183	Mobility reversal of polyelectrolyte-grafted colloids in monovalent salt solutions. *Physical Review Letters*, **2014**, 113, 238301	7.4	23
182	Origin of current blockades in nanopore translocation experiments. *Physical Review Letters*, **2014**, 112, 018101	7.4	38
181	Communication: Kinetic and pairing contributions in the dielectric spectra of electrolyte solutions. *Journal of Chemical Physics*, **2014**, 140, 211101	3.9	22
180	Simulation of electric double layers around charged colloids in aqueous solution of variable permittivity. *Journal of Chemical Physics*, **2014**, 141, 064902	3.9	25
179	The solvation and ion condensation properties for sulfonated polyelectrolytes in different solvents□ computational study. *New Journal of Physics*, **2014**, 16, 025001	2.9	35
178	ESPResSo 3.1: Molecular Dynamics Software for Coarse-Grained Models. *Lecture Notes in Computational Science and Engineering*, **2013**, 1-23	0.3	90
177	Complex tracer diffusion dynamics in polymer solutions. *Physical Review Letters*, **2013**, 111, 088301	7.4	48
176	Refining classical force fields for ionic liquids: theory and application to [MMIM][Cl]. *Physical Chemistry Chemical Physics*, **2013**, 15, 2037-49	3.6	19
175	Cluster formation in systems of shifted-dipole particles. *Soft Matter*, **2013**, 9, 3535	3.6	32
174	Phase diagram for a single flexible Stockmayer polymer at zero field. *Soft Matter*, **2013**, 9, 7185	3.6	25
173	Comparison of scalable fast methods for long-range interactions. *Physical Review E*, **2013**, 88, 063308	2.4	58
172	Vapor-liquid coexistence of the Stockmayer fluid in nonuniform external fields. *Physical Review E*, **2013**, 87, 052128	2.4	6
171	Electrophoretic mobility and charge inversion of a colloidal particle studied by single-colloid electrophoresis and molecular dynamics simulations. *Physical Review E*, **2013**, 87, 022302	2.4	50
170	Effects of the dipolar interaction on the equilibrium morphologies of a single supramolecular magnetic filament in bulk. *Journal of Chemical Physics*, **2013**, 139, 044904	3.9	27
169	Electrophoretic mobility reversal of polyampholytes induced by strong electric fields or confinement. *Journal of Chemical Physics*, **2013**, 138, 194905	3.9	12

168	Efficient Algorithms for Electrostatic Interactions Including Dielectric Contrasts. *Entropy*, **2013**, 15, 4569-4588	1.5	35
167	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	3.9	22
166	Molecular Simulations of Hydrogels **2013**, 205-221		11
165	Tracer diffusion in a crowded cylindrical channel. *Physical Review E*, **2013**, 87, 062709	2.4	18
164	Seawater Desalination via Hydrogels: Practical Realisation and First Coarse Grained Simulations **2013**, 247-263		15
163	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	10
162	Magnetic Flux Topology of 2D Point Dipoles. *Computer Graphics Forum*, **2012**, 31, 955-964	2.4	8
161	Deformation mechanisms in 2D magnetic gels studied by computer simulations. *Soft Matter*, **2012**, 8, 9923	3.6	74
160	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, 11425-32	3.6	12
159	How to Convert SPME to P3M: Influence Functions and Error Estimates. *Journal of Chemical Theory and Computation*, **2012**, 8, 936-47	6.4	21
158	Modeling the Structure and Dynamics of Polyelectrolyte Multilayers **2012**, 121-166		3
157	Ionic liquids studied across different scales: a computational perspective. *Faraday Discussions*, **2012**, 154, 111-32; discussion 189-220, 465-71	3.6	86
156	Effects of dielectric mismatch and chain flexibility on the translocation barriers of charged macromolecules through solid state nanopores. *Soft Matter*, **2012**, 8, 9480	3.6	10
155	Force fields for studying the structure and dynamics of ionic liquids: a critical review of recent developments. *ChemPhysChem*, **2012**, 13, 1625-37	3.2	218
154	Multiscale approaches and perspectives to modeling aqueous electrolytes and polyelectrolytes. *Topics in Current Chemistry*, **2012**, 307, 251-94		8
153	Microstructure of Bidisperse Ferrofluids in a Monolayer. *Solid State Phenomena*, **2012**, 190, 625-628	0.4	2
152	Influence of Charged Polymer Coatings on Electro-Osmotic Flow: Molecular Dynamics Simulations. *Macromolecules*, **2011**, 44, 9455-9463	5.5	27
151	Atomistic Study of Surface Effects on Polyelectrolyte Adsorption: Case Study of a Poly(styrenesulfonate) Monolayer. *Macromolecules*, **2011**, 44, 1707-1718	5.5	28

150	Locality and Fluctuations: Trends in Imidazolium-Based Ionic Liquids and Beyond. *Journal of Chemical Theory and Computation*, **2011**, 7, 3040-4	6.4	80
149	Simulational study of anomalous tracer diffusion in hydrogels. *Colloid and Polymer Science*, **2011**, 289, 523-534	2.4	26
148	Removal of spurious self-interactions in particle-mesh methods. *Computer Physics Communications*, **2011**, 182, 1919-1923	4.2	7
147	Hydrogels in Poor Solvents: A Molecular Dynamics Study. *Macromolecular Theory and Simulations*, **2011**, 20, 721-734	1.5	41
146	Novel Simulation Approaches for Polymeric and Soft Matter Systems. *Macromolecular Theory and Simulations*, **2011**, 20, 444-445	1.5	0
145	Semiflexible magnetic filaments near attractive flat surfaces: a Langevin dynamics study. *Soft Matter*, **2011**, 7, 1809-1818	3.6	15
144	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, 16336-42	3.6	19
143	Ferrofluids with shifted dipoles: ground state structures. *Soft Matter*, **2011**, 7, 5217	3.6	44
142	Applying ICC? to DNA translocation: Effect of dielectric boundaries. *Computer Physics Communications*, **2011**, 182, 33-35	4.2	17
141	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	2.8	3
140	Structure factor of ferrofluids with chain aggregates: Theory and computer simulations. *Journal of Magnetism and Magnetic Materials*, **2011**, 323, 1263-1268	2.8	12
139	Magnetic particles with shifted dipoles. *Journal of Magnetism and Magnetic Materials*, **2011**, 323, 1269-1272	2.8	18
138	Ground state structures in ferrofluid monolayers. *Journal of Magnetism and Magnetic Materials*, **2011**, 323, 1298-1301	2.8	10
137	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	3.9	32
136	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	3.9	5
135	An iterative, fast, linear-scaling method for computing induced charges on arbitrary dielectric boundaries. *Journal of Chemical Physics*, **2010**, 132, 154112	3.9	61
134	Optimizing working parameters of the smooth particle mesh Ewald algorithm in terms of accuracy and efficiency. *Journal of Chemical Physics*, **2010**, 133, 034117	3.9	78
133	Interlaced P3M algorithm with analytical and ik-differentiation. *Journal of Chemical Physics*, **2010**, 132, 234103	3.9	22

132	Implicit method for simulating electrohydrodynamics of polyelectrolytes. *Physical Review Letters*, **2010**, 105, 148301	7.4	21
131	Equilibrium polyelectrolyte bundles with different multivalent counterion concentrations. *Physical Review E*, **2010**, 82, 031901	2.4	20
130	Poly(styrenesulfonate)–Poly(diallyldimethylammonium) Mixtures: Toward the Understanding of Polyelectrolyte Complexes and Multilayers via Atomistic Simulations. *Macromolecules*, **2010**, 43, 7828-7838	5.5	40
129	Ionic charge reduction and atomic partial charges from first-principles calculations of 1,3-dimethylimidazolium chloride. *Journal of Physical Chemistry B*, **2010**, 114, 6150-5	3.4	109
128	Mesoscale modelling of polyelectrolyte electrophoresis. *Faraday Discussions*, **2010**, 144, 57-70; discussion 93-110, 467-81	3.6	27
127	Electrostatic properties of liquid 1,3-dimethylimidazolium chloride: role of local polarization and effect of the bulk. *Physical Chemistry Chemical Physics*, **2010**, 12, 1817-21	3.6	34
126	Behavior of bulky ferrofluids in the diluted low-coupling regime: theory and simulation. *Physical Review E*, **2010**, 81, 011501	2.4	24
125	Bidisperse monolayers: Theory and computer simulations. *Physics Procedia*, **2010**, 9, 87-90		3
124	Towards multiscale modeling of ionic liquids: From electronic structure to bulk properties. *Journal of Molecular Liquids*, **2010**, 152, 2-8	6	46
123	Ground state structures in ferrofluid monolayers. *Physical Review E*, **2009**, 80, 031404	2.4	59
122	Comparison of a hydrogel model to the Poisson-Boltzmann cell model. *Journal of Chemical Physics*, **2009**, 131, 094903	3.9	65
121	Ensemble inequivalence in single-molecule experiments. *Physical Review E*, **2009**, 79, 051118	2.4	20
120	Modeling the separation of macromolecules: a review of current computer simulation methods. *Electrophoresis*, **2009**, 30, 792-818	3.6	116
119	Modeling strategies for polyelectrolyte multilayers. *European Physical Journal: Special Topics*, **2009**, 177, 129-148	2.3	11
118	Optimizing End-Labeled Free-Solution Electrophoresis by Increasing the Hydrodynamic Friction of the Drag Tag. *Macromolecules*, **2009**, 42, 5352-5359	5.5	11
117	Understanding polyelectrolyte multilayers: an open challenge for simulations. *Soft Matter*, **2009**, 5, 4412	3.6	51
116	Polyelectrolytes in electric fields: measuring the dynamical effective charge and effective friction. *Soft Matter*, **2009**, 5, 2079	3.6	58
115	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	27

114	Mesoscopic simulations of the counterion-induced electro-osmotic flow: a comparative study. *Journal of Chemical Physics*, **2009**, 130, 244702	3.9	45
113	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	3.9	81
112	Effect of anions on static orientational correlations, hydrogen bonds, and dynamics in ionic liquids: a simulational study. *Journal of Physical Chemistry B*, **2008**, 112, 1743-51	3.4	105
111	Importance of hydrodynamic shielding for the dynamic behavior of short polyelectrolyte chains. *Physical Review Letters*, **2008**, 100, 096104	7.4	75
110	On the importance of hydrodynamic interactions in polyelectrolyte electrophoresis. *Journal of Physics Condensed Matter*, **2008**, 20, 494217	1.8	5
109	P3M algorithm for dipolar interactions. *Journal of Chemical Physics*, **2008**, 129, 234104	3.9	69
108	Microstructure analysis of monodisperse ferrofluid monolayers: theory and simulation. *Physical Chemistry Chemical Physics*, **2008**, 10, 1883-95	3.6	47
107	Colloidal electrophoresis: scaling analysis, GreenKubo relation, and numerical results. *Journal of Physics Condensed Matter*, **2008**, 20, 404214	1.8	25
106	Aggregate formation in ferrofluid monolayers: simulations and theory. *Journal of Physics Condensed Matter*, **2008**, 20, 204125	1.8	26
105	The optimal P3M algorithm for computing electrostatic energies in periodic systems. *Journal of Chemical Physics*, **2008**, 128, 034109	3.9	20
104	Study of 1,3-dimethylimidazolium chloride with electronic structure methods and force field approaches. *Journal of Chemical Physics*, **2008**, 129, 174503	3.9	32
103	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	3.9	34
102	Shear effects on crystal nucleation in colloidal suspensions. *Physical Review E*, **2008**, 78, 031403	2.4	32
101	Simulation of charge reversal in salty environments: giant overcharging?. *European Physical Journal E*, **2008**, 26, 191-5	1.5	39
100	Interactions of like-charged rods at low temperatures: analytical theory vs. simulations. *European Physical Journal E*, **2008**, 27, 21-9	1.5	12
99	Electrophoresis of colloidal dispersions in the low-salt regime. *Physical Review Letters*, **2007**, 98, 176105	7.4	110
98	Osmotic Coefficient Calculations for Dilute Solutions of Short Stiff-Chain Polyelectrolytes. *Macromolecules*, **2007**, 40, 731-738	5.5	22
97	Stability of Hydrophobically Modified Poly(p-phenylenesulfonate) Bundles As Observed by Molecular Dynamics Simulation. *Macromolecules*, **2007**, 40, 1703-1707	5.5	9

96	Finite-size polyelectrolyte bundles at thermodynamic equilibrium. *Europhysics Letters*, **2007**, 77, 16001	1.6	32
95	Magnetic properties of polydisperse ferrofluids: a critical comparison between experiment, theory, and computer simulation. *Physical Review E*, **2007**, 75, 061405	2.4	110
94	ICMMM2D: an accurate method to include planar dielectric interfaces via image charge summation. *Journal of Chemical Physics*, **2007**, 127, 154723	3.9	31
93	Controlled DNA compaction within chromatin: The tail-bridging effect. *Europhysics Letters*, **2006**, 73, 135-141	1.6	30
92	Equilibrium properties of a bidisperse ferrofluid with chain aggregates: theory and computer simulations. *Journal of Physics Condensed Matter*, **2006**, 18, S2737-S2756	1.8	36
91	The Osmotic Behavior of Short Stiff Polyelectrolytes. *Macromolecular Symposia*, **2006**, 245-246, 297-306	0.8	3
90	Optimal cell approach to osmotic properties of finite stiff-chain polyelectrolytes. *Physical Review Letters*, **2006**, 96, 088302	7.4	28
89	Tail-induced attraction between nucleosome core particles. *Physical Review E*, **2006**, 74, 031919	2.4	36
88	Simulating Charged Systems with ESPResSo **2006**, 193-221		2
87	Modeling multibody effects in ionic solutions with a concentration dependent dielectric permittivity. *Physical Review Letters*, **2006**, 96, 147801	7.4	104
86	Osmotic coefficients of atomistic NaCl (aq) force fields. *Journal of Chemical Physics*, **2006**, 124, 164509	3.9	122
85	The Swelling Behavior of Charged Hydrogels. *Macromolecular Symposia*, **2006**, 237, 90-107	0.8	42
84	Polydispersity Influence upon Magnetic Properties of Aggregated Ferrofluids. *Zeitschrift Fur Physikalische Chemie*, **2006**, 220, 105-115	3.1	2
83	ESPResSo□n extensible simulation package for research on soft matter systems. *Computer Physics Communications*, **2006**, 174, 704-727	4.2	544
82	Spatial distribution of polyelectrolyte and counterions in nanocapsules: a computer simulation study. *Physical Review E*, **2006**, 73, 021801	2.4	19
81	Swelling of polyelectrolyte networks. *Journal of Chemical Physics*, **2005**, 122, 154903	3.9	84
80	Structure and magnetic properties of mono- and bi-dispersed ferrofluids as revealed by simulations. *Journal of Magnetism and Magnetic Materials*, **2005**, 289, 234-237	2.8	18
79	The structure of ferrofluids: A status report. *Current Opinion in Colloid and Interface Science*, **2005**, 10, 133-140	7.6	191

78	Computer Simulations of the Hairy Rod Model. *Macromolecular Chemistry and Physics*, **2005**, 206, 77-82	2.6	17
77	Incorporation of excluded-volume correlations into Poisson-Boltzmann theory. *Physical Review E*, **2005**, 71, 061106	2.4	71
76	Computer simulations of the structure of colloidal ferrofluids. *Physical Review E*, **2005**, 71, 061203	2.4	54
75	MMM1D: a method for calculating electrostatic interactions in one-dimensional periodic geometries. *Journal of Chemical Physics*, **2005**, 123, 144103	3.9	37
74	The Physics of Overcharging **2005**, 475-488		1
73	Polyelectrolyte bundles. *Journal of Physics Condensed Matter*, **2004**, 16, S2135-S2144	1.8	24
72	Screening of spherical colloids beyond mean field: a local density functional approach. *Physical Review E*, **2004**, 69, 051401	2.4	13
71	Magnetization of polydisperse colloidal ferrofluids: effect of magnetostriction. *Physical Review E*, **2004**, 70, 061404	2.4	12
70	Attraction and unbinding of like-charged rods. *Europhysics Letters*, **2004**, 67, 130-136	1.6	52
69	Scaling in polyelectrolyte networks. *Europhysics Letters*, **2004**, 67, 786-792	1.6	60
68	Polyelectrolyte adsorption and multilayering on charged colloidal particles. *Journal of Polymer Science, Part B: Polymer Physics*, **2004**, 42, 3557-3570	2.6	34
67	Applying the chain formation model to magnetic properties of aggregated ferrofluids. *Physical Review E*, **2004**, 69, 031206	2.4	43
66	Electrophoretic mobility of a charged colloidal particle: a computer simulation study. *Journal of Physics Condensed Matter*, **2004**, 16, S4063-S4073	1.8	68
65	Conformations and solution structure of polyelectrolytes in poor solvent. *Macromolecular Symposia* , **2004**, 211, 43-54	0.8	17
64	Poor-solvent polyelectrolytes. *Journal of Physics Condensed Matter*, **2003**, 15, S205-S211	1.8	10
63	Polyelectrolyte Multilayering on a Charged Sphere. *Langmuir*, **2003**, 19, 4473-4482	4	71
62	Boundary condition effects in the simulation study of equilibrium properties of magnetic dipolar fluids. *Journal of Chemical Physics*, **2003**, 119, 379-387	3.9	39
61	Structure and magnetic properties of polydisperse ferrofluids: a molecular dynamics study. *Physical Review E*, **2003**, 68, 041401	2.4	116

60	Single-Chain Properties of Polyelectrolytes in Poor Solvent. *Journal of Physical Chemistry B*, **2003**, 107, 8041-8055	3.4	129
59	Attraction and Ionic Correlations between Charged Stiff Polyelectrolytes. *Macromolecules*, **2003**, 36, 249-259	5.5	75
58	Ion pairing in model electrolytes: A study via three-particle correlation functions. *Journal of Chemical Physics*, **2003**, 119, 4842-4856	3.9	11
57	Conformational properties of poor solvent polyelectrolytes. *Computer Physics Communications*, **2002**, 147, 321-324	4.2	44
56	Charge inversion in colloidal systems. *Computer Physics Communications*, **2002**, 147, 282-285	4.2	15
55	MMM2D: A fast and accurate summation method for electrostatic interactions in 2D slab geometries. *Computer Physics Communications*, **2002**, 148, 327-348	4.2	69
54	A novel method for calculating electrostatic interactions in 2D periodic slab geometries. *Chemical Physics Letters*, **2002**, 354, 324-330	2.5	36
53	Conformation of a polyelectrolyte complexed to a like-charged colloid. *Physical Review E*, **2002**, 65, 041805	2.4	20
52	Electrostatics in periodic slab geometries. II. *Journal of Chemical Physics*, **2002**, 117, 2503-2512	3.9	64
51	Structure of polyelectrolytes in poor solvent. *Europhysics Letters*, **2002**, 60, 566-572	1.6	85
50	Overcharging: The crucial role of excluded volume. *Europhysics Letters*, **2002**, 60, 383-389	1.6	88
49	Molecular dynamics study on the equilibrium magnetization properties and structure of ferrofluids. *Physical Review E*, **2002**, 66, 021405	2.4	184
48	Like-charge colloid–polyelectrolyte complexation. *Journal of Chemical Physics*, **2002**, 117, 2947-2960	3.9	36
47	Electrostatics in periodic slab geometries. I. *Journal of Chemical Physics*, **2002**, 117, 2496-2502	3.9	135
46	Theory and simulations of rigid polyelectrolytes. *Molecular Physics*, **2002**, 100, 2941-2956	1.7	37
45	The osmotic coefficient of rod-like polyelectrolytes: Computer simulation, analytical theory, and experiment. *European Physical Journal E*, **2001**, 5, 97-103	1.5	48
44	Effect of colloidal charge discretization in the primitive model. *European Physical Journal E*, **2001**, 4, 363-370	1.5	46
43	End effects of strongly charged polyelectrolytes: A molecular dynamics study. *Journal of Chemical Physics*, **2001**, 114, 9674-9682	3.9	59

42	Strong electrostatic interactions in spherical colloidal systems. *Physical Review E*, **2001**, 64, 021405	2.4	63
41	Estimate of the cutoff errors in the Ewald summation for dipolar systems. *Journal of Chemical Physics*, **2001**, 115, 6351-6359	3.9	87
40	Overcharging of DNA in the Presence of Salt: Theory and Simulation. *Journal of Physical Chemistry B*, **2001**, 105, 10983-10991	3.4	113
39	Computer Simulations of Charged Systems **2001**, 117-148		2
38	Cell Model and Poisson-Boltzmann Theory: A Brief Introduction **2001**, 27-52		26
37	A stable local density functional approach to ion-ion correlations. *Europhysics Letters*, **2000**, 52, 80-86	1.6	63
36	Ground state of two unlike charged colloids: An analogy with ionic bonding. *Europhysics Letters*, **2000**, 51, 461-467	1.6	36
35	Strong attraction between charged spheres due to metastable ionized states. *Physical Review Letters*, **2000**, 85, 872-5	7.4	123
34	Fraction of Condensed Counterions around a Charged Rod: Comparison of Poisson-Boltzmann Theory and Computer Simulations. *Macromolecules*, **2000**, 33, 199-206	5.5	251
33	SIMPLICIAL QUANTUM GRAVITY ON A RANDOMLY TRIANGULATED SPHERE. *International Journal of Modern Physics A*, **1999**, 14, 3885-3903	1.2	2
32	Z2-Regge versus standard Regge calculus in two dimensions. *Physical Review D*, **1999**, 59,	4.9	2
31	Strongly Charged, Flexible Polyelectrolytes in Poor Solvents: Molecular Dynamics Simulations *Langmuir*, **1999**, 15, 4033-4044	4	207
30	How to mesh up Ewald sums. II. An accurate error estimate for the particle-particle-particle-mesh algorithm. *Journal of Chemical Physics*, **1998**, 109, 7694-7701	3.9	238
29	Standard and Z2-Regge theory in two dimensions. *Nuclear Physics, Section B, Proceedings Supplements*, **1998**, 63, 769-771		2
28	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	3.9	493
27	Critical Exponents of the Classical Heisenberg Ferromagnet. *Physical Review Letters*, **1997**, 78, 2265-2265	7.4	14
26	Monte Carlo study of asymmetric 2D XY model. *Physica A: Statistical Mechanics and Its Applications*, **1997**, 246, 633-645	3.3	7
25	Fixed versus random triangulations in 2D Regge calculus. *Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics*, **1997**, 390, 59-63	4.2	6

24	Influence of the Path Integral Measure in Quantum Gravity. *NATO ASI Series Series B: Physics*, **1997**, 417-417		
23	Measuring the string susceptibility in 2D simplicial quantum gravity using the Regge approach. *Nuclear Physics B*, **1996**, 477, 465-488	2.8	9
22	New results on □tr in 2D quantum gravity using Regge calculus. *Nuclear Physics, Section B, Proceedings Supplements*, **1996**, 47, 621-624		1
21	Ising spins on a gravitating sphere. *Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics*, **1996**, 375, 69-74	4.2	18
20	Measure dependence of 2D simplicial quantum gravity. *Nuclear Physics, Section B, Proceedings Supplements*, **1995**, 42, 722-724		4
19	The Ising transition in 2D simplicial quantum gravity □can Regge calculus be right?. *Nuclear Physics, Section B, Proceedings Supplements*, **1995**, 42, 725-727		3
18	HIGH-PRECISION MONTE CARLO DETERMINATION OF □IN THE 3D CLASSICAL HEISENBERG MODEL. *International Journal of Modern Physics C*, **1994**, 05, 267-270	1.1	
17	Monte Carlo study of topological defects in the 3D Heisenberg model. *Journal of Physics A*, **1994**, 27, 2553-2563		34
16	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	4.2	31
15	Are defects important for 3D phase transitions?. *Nuclear Physics, Section B, Proceedings Supplements*, **1994**, 34, 692-694		
14	Critical exponents of the classical three-dimensional Heisenberg model: A single-cluster Monte Carlo study. *Physical Review B*, **1993**, 48, 936-950	3.3	174
13	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	2.3	49
12	High-temperature series analyses of the classical Heisenberg and XY models. *Physica A: Statistical Mechanics and Its Applications*, **1993**, 201, 581-592	3.3	40
11	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		8
10	Connections in Bergmann manifolds. *International Journal of Theoretical Physics*, **1990**, 29, 23-36	1.1	4
9	Neutrino spectrum of Einstein universes. *Journal of Mathematical Physics*, **1988**, 29, 2273-2279	1.2	4
8	The hyperspin structure of unitary groups. *Journal of Mathematical Physics*, **1988**, 29, 978-986	1.2	7
7	Hypergravitational field equations. *Physical Review Letters*, **1987**, 59, 1265-1266	7.4	7

6	Christoffel formula and geodesic motion in hyperspin manifolds. *International Journal of Theoretical Physics*, **1986**, 25, 1209-1213	1.1	13
5	Hyperspin manifolds. *International Journal of Theoretical Physics*, **1986**, 25, 441-463	1.1	22
4	Elementary explanation of boundary shading in chaotic-attractor plots for the Feigenbaum map and the circle map. *Physical Review A*, **1986**, 33, 2809-2812	2.6	7
3	Efficient Methods to Compute Long-Range Interactions for Soft Matter Systems59-109		27
2	Stiff-Chain Polyelectrolytes. *Advances in Polymer Science*,1-27	1.3	42
1	Polyelectrolyte Theory. *Advances in Polymer Science*,67-111	1.3	133