Christian Holm

List of Publications by Citations

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	ESPResSo—an extensible simulation package for research on soft matter systems. *Computer Physics Communications*, **2006**, 174, 704-727	4.2	544
292	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
291	Fraction of Condensed Counterions around a Charged Rod: Comparison of Poisson−Boltzmann Theory and Computer Simulations. *Macromolecules*, **2000**, 33, 199-206	5.5	251
290	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
289	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
288	Strongly Charged, Flexible Polyelectrolytes in Poor Solvents: Molecular Dynamics Simulations *Langmuir*, **1999**, 15, 4033-4044	4	207
287	The structure of ferrofluids: A status report. *Current Opinion in Colloid and Interface Science*, **2005**, 10, 133-140	7.6	191
286	Molecular dynamics study on the equilibrium magnetization properties and structure of ferrofluids. *Physical Review E*, **2002**, 66, 021405	2.4	184
285	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
284	Electrostatics in periodic slab geometries. I. *Journal of Chemical Physics*, **2002**, 117, 2496-2502	3.9	135
283	Polyelectrolyte Theory. *Advances in Polymer Science*,67-111	1.3	133
282	Single-Chain Properties of Polyelectrolytes in Poor Solvent *Journal of Physical Chemistry B*, **2003**, 107, 8041-8055	3.4	129
281	Strong attraction between charged spheres due to metastable ionized states. *Physical Review Letters*, **2000**, 85, 872-5	7.4	123
280	Osmotic coefficients of atomistic NaCl (aq) force fields. *Journal of Chemical Physics*, **2006**, 124, 164509	3.9	122
279	Modeling the separation of macromolecules: a review of current computer simulation methods. *Electrophoresis*, **2009**, 30, 792-818	3.6	116
278	Structure and magnetic properties of polydisperse ferrofluids: a molecular dynamics study. *Physical Review E*, **2003**, 68, 041401	2.4	116
277	Overcharging of DNA in the Presence of Salt: Theory and Simulation. *Journal of Physical Chemistry B*, **2001**, 105, 10983-10991	3.4	113

276	Electrophoresis of colloidal dispersions in the low-salt regime. *Physical Review Letters*, **2007**, 98, 176105	7.4	110
275	Magnetic properties of polydisperse ferrofluids: a critical comparison between experiment, theory, and computer simulation. *Physical Review E*, **2007**, 75, 061405	2.4	110
274	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
273	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
272	Modeling multibody effects in ionic solutions with a concentration dependent dielectric permittivity. *Physical Review Letters*, **2006**, 96, 147801	7.4	104
271	ESPResSo 3.1: Molecular Dynamics Software for Coarse-Grained Models. *Lecture Notes in Computational Science and Engineering*, **2013**, 1-23	0.3	90
270	Overcharging: The crucial role of excluded volume. *Europhysics Letters*, **2002**, 60, 383-389	1.6	88
269	Estimate of the cutoff errors in the Ewald summation for dipolar systems. *Journal of Chemical Physics*, **2001**, 115, 6351-6359	3.9	87
268	Ionic liquids studied across different scales: a computational perspective. *Faraday Discussions*, **2012**, 154, 111-32; discussion 189-220, 465-71	3.6	86
267	Structure of polyelectrolytes in poor solvent. *Europhysics Letters*, **2002**, 60, 566-572	1.6	85
266	Swelling of polyelectrolyte networks. *Journal of Chemical Physics*, **2005**, 122, 154903	3.9	84
265	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
264	Locality and Fluctuations: Trends in Imidazolium-Based Ionic Liquids and Beyond. *Journal of Chemical Theory and Computation*, **2011**, 7, 3040-4	6.4	80
263	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
262	Importance of hydrodynamic shielding for the dynamic behavior of short polyelectrolyte chains. *Physical Review Letters*, **2008**, 100, 096104	7.4	75
261	Attraction and Ionic Correlations between Charged Stiff Polyelectrolytes. *Macromolecules*, **2003**, 36, 249-259	5.5	75
260	Ionic screening and dissociation are crucial for understanding chemical self-propulsion in polar solvents. *Soft Matter*, **2017**, 13, 1200-1222	3.6	74
259	Deformation mechanisms in 2D magnetic gels studied by computer simulations. *Soft Matter*, **2012**, 8, 9923	3.6	74

258	Polyelectrolyte Multilayering on a Charged Sphere. *Langmuir*, **2003**, 19, 4473-4482	4	71
257	Incorporation of excluded-volume correlations into Poisson-Boltzmann theory. *Physical Review E*, **2005**, 71, 061106	2.4	71
256	P3M algorithm for dipolar interactions. *Journal of Chemical Physics*, **2008**, 129, 234104	3.9	69
255	MMM2D: A fast and accurate summation method for electrostatic interactions in 2D slab geometries. *Computer Physics Communications*, **2002**, 148, 327-348	4.2	69
254	Electrophoretic mobility of a charged colloidal particle: a computer simulation study. *Journal of Physics Condensed Matter*, **2004**, 16, S4063-S4073	1.8	68
253	Comparison of a hydrogel model to the Poisson-Boltzmann cell model. *Journal of Chemical Physics*, **2009**, 131, 094903	3.9	65
252	Electrostatics in periodic slab geometries. II. *Journal of Chemical Physics*, **2002**, 117, 2503-2512	3.9	64
251	Strong electrostatic interactions in spherical colloidal systems. *Physical Review E*, **2001**, 64, 021405	2.4	63
250	A stable local density functional approach to ion-ion correlations. *Europhysics Letters*, **2000**, 52, 80-86	1.6	63
249	ESPResSo 4.0 an extensible software package for simulating soft matter systems. *European Physical Journal: Special Topics*, **2019**, 227, 1789-1816	2.3	62
248	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
247	An iterative, fast, linear-scaling method for computing induced charges on arbitrary dielectric boundaries. *Journal of Chemical Physics*, **2010**, 132, 154112	3.9	61
246	Scaling in polyelectrolyte networks. *Europhysics Letters*, **2004**, 67, 786-792	1.6	60
245	Buckling of paramagnetic chains in soft gels. *Soft Matter*, **2016**, 12, 228-37	3.6	59
244	Ground state structures in ferrofluid monolayers. *Physical Review E*, **2009**, 80, 031404	2.4	59
243	End effects of strongly charged polyelectrolytes: A molecular dynamics study. *Journal of Chemical Physics*, **2001**, 114, 9674-9682	3.9	59
242	Comparison of scalable fast methods for long-range interactions. *Physical Review E*, **2013**, 88, 063308	2.4	58
241	Polyelectrolytes in electric fields: measuring the dynamical effective charge and effective friction. *Soft Matter*, **2009**, 5, 2079	3.6	58

240	Modeling of Polyelectrolyte Gels in Equilibrium with Salt Solutions. *Macromolecules*, **2015**, 48, 7698-7708	5.5	57
239	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
238	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
237	Charge Me Slowly, I Am in a Hurry: Optimizing Charge-Discharge Cycles in Nanoporous Supercapacitors. *ACS Nano*, **2018**, 12, 9733-9741	16.7	54
236	Computer simulations of the structure of colloidal ferrofluids. *Physical Review E*, **2005**, 71, 061203	2.4	54
235	Attraction and unbinding of like-charged rods. *Europhysics Letters*, **2004**, 67, 130-136	1.6	52
234	Polymer architecture of magnetic gels: a review. *Journal of Physics Condensed Matter*, **2018**, 30, 063002	1.8	51
233	Understanding polyelectrolyte multilayers: an open challenge for simulations. *Soft Matter*, **2009**, 5, 4412	3.6	51
232	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
231	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
230	Complex tracer diffusion dynamics in polymer solutions. *Physical Review Letters*, **2013**, 111, 088301	7.4	48
229	The osmotic coefficient of rod-like polyelectrolytes: Computer simulation, analytical theory, and experiment. *European Physical Journal E*, **2001**, 5, 97-103	1.5	48
228	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
227	Microstructure analysis of monodisperse ferrofluid monolayers: theory and simulation. *Physical Chemistry Chemical Physics*, **2008**, 10, 1883-95	3.6	47
226	Towards multiscale modeling of ionic liquids: From electronic structure to bulk properties. *Journal of Molecular Liquids*, **2010**, 152, 2-8	6	46
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224	Mesoscopic simulations of the counterion-induced electro-osmotic flow: a comparative study. *Journal of Chemical Physics*, **2009**, 130, 244702	3.9	45
223	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

222	Ferrofluids with shifted dipoles: ground state structures. *Soft Matter*, **2011**, 7, 5217	3.6	44
221	Conformational properties of poor solvent polyelectrolytes. *Computer Physics Communications*, **2002**, 147, 321-324	4.2	44
220	Applying the chain formation model to magnetic properties of aggregated ferrofluids. *Physical Review E*, **2004**, 69, 031206	2.4	43
219	The Swelling Behavior of Charged Hydrogels. *Macromolecular Symposia*, **2006**, 237, 90-107	0.8	42
218	Stiff-Chain Polyelectrolytes. *Advances in Polymer Science*,1-27	1.3	42
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216	Electrode Models for Ionic Liquid-Based Capacitors. *Journal of Physical Chemistry C*, **2015**, 119, 22445-22451	3.3	41
215	Hydrogels in Poor Solvents: A Molecular Dynamics Study. *Macromolecular Theory and Simulations*, **2011**, 20, 721-734	1.5	41
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213	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
212	Simulation of charge reversal in salty environments: giant overcharging?. *European Physical Journal E*, **2008**, 26, 191-5	1.5	39
211	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
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209	Origin of current blockades in nanopore translocation experiments. *Physical Review Letters*, **2014**, 112, 018101	7.4	38
208	MMM1D: a method for calculating electrostatic interactions in one-dimensional periodic geometries. *Journal of Chemical Physics*, **2005**, 123, 144103	3.9	37
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206	Microfluidic pumping by micromolar salt concentrations. *Soft Matter*, **2017**, 13, 1505-1518	3.6	36
205	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

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203	Tail-induced attraction between nucleosome core particles. *Physical Review E*, **2006**, 74, 031919	2.4	36
202	A novel method for calculating electrostatic interactions in 2D periodic slab geometries. *Chemical Physics Letters*, **2002**, 354, 324-330	2.5	36
201	Like-charge colloid–polyelectrolyte complexation. *Journal of Chemical Physics*, **2002**, 117, 2947-2960	3.9	36
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195	Polyelectrolyte adsorption and multilayering on charged colloidal particles. *Journal of Polymer Science, Part B: Polymer Physics*, **2004**, 42, 3557-3570	2.6	34
194	Monte Carlo study of topological defects in the 3D Heisenberg model. *Journal of Physics A*, **1994**, 27, 2553-2563		34
193	Machine-learned interatomic potentials by active learning: amorphous and liquid hafnium dioxide. *Npj Computational Materials*, **2020**, 6,	10.9	34
192	Cluster formation in systems of shifted-dipole particles. *Soft Matter*, **2013**, 9, 3535	3.6	32
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176	Optimal cell approach to osmotic properties of finite stiff-chain polyelectrolytes. *Physical Review Letters*, **2006**, 96, 088302	7.4	28
175	A self-consistent mean-field model for polyelectrolyte gels. *Soft Matter*, **2017**, 13, 3264-3274	3.6	27
174	Diffusiophoretic self-propulsion for partially catalytic spherical colloids. *IEEE Transactions on Nanobioscience*, **2015**, 14, 272-88	3.4	27
173	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
172	Influence of Charged Polymer Coatings on Electro-Osmotic Flow: Molecular Dynamics Simulations. *Macromolecules*, **2011**, 44, 9455-9463	5.5	27
171	Mesoscale modelling of polyelectrolyte electrophoresis. *Faraday Discussions*, **2010**, 144, 57-70; discussion 93-110, 467-81	3.6	27
170	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
169	Efficient Methods to Compute Long-Range Interactions for Soft Matter Systems59-109		27

168	Simulational study of anomalous tracer diffusion in hydrogels. *Colloid and Polymer Science*, **2011**, 289, 523-534	2.4	26
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166	Cell Model and Poisson-Boltzmann Theory: A Brief Introduction **2001**, 27-52		26
165	Properties of Apolar Solutes in Alkyl Imidazolium-Based Ionic Liquids: The Importance of Local Interactions. *ChemPhysChem*, **2016**, 17, 387-94	3.2	26
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162	Simulation of electric double layers around charged colloids in aqueous solution of variable permittivity. *Journal of Chemical Physics*, **2014**, 141, 064902	3.9	25
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158	Behavior of bulky ferrofluids in the diluted low-coupling regime: theory and simulation. *Physical Review E*, **2010**, 81, 011501	2.4	24
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156	Understanding the onset of oscillatory swimming in microchannels. *Soft Matter*, **2016**, 12, 4704-8	3.6	24
155	Properties of the polarizable MARTINI water model: A comparative study for aqueous electrolyte solutions. *Journal of Molecular Liquids*, **2015**, 212, 103-110	6	23
154	Mobility reversal of polyelectrolyte-grafted colloids in monovalent salt solutions. *Physical Review Letters*, **2014**, 113, 238301	7.4	23
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152	The Raspberry model for hydrodynamic interactions revisited. II. The effect of confinement. *Journal of Chemical Physics*, **2015**, 143, 084108	3.9	22
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150	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
149	Interlaced P3M algorithm with analytical and ik-differentiation. *Journal of Chemical Physics*, **2010**, 132, 234103	3.9	22
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