Jens Smiatek

List of Publications by Citations

99 papers	1,934 citations	27 h-index	37 g-index
101 ext. papers	2,238 ext. citations	4.1 avg, IF	5.86 L-index

#	Paper	IF	Citations
99	Properties of compatible solutes in aqueous solution. *Biophysical Chemistry*, **2012**, 160, 62-8	3.5	64
98	Aqueous ionic liquids and their effects on protein structures: an overview on recent theoretical and experimental results. *Journal of Physics Condensed Matter*, **2017**, 29, 233001	1.8	62
97	Osmolyte effects: impact on the aqueous solution around charged and neutral spheres. *Journal of Physical Chemistry B*, **2014**, 118, 771-82	3.4	60
96	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
95	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
94	Stabilizing effect of TMAO on globular PNIPAM states: preferential attraction induces preferential hydration. *Physical Chemistry Chemical Physics*, **2016**, 18, 31459-31470	3.6	51
93	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
92	Mesoscopic simulations of the counterion-induced electro-osmotic flow: a comparative study. *Journal of Chemical Physics*, **2009**, 130, 244702	3.9	45
91	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
90	Tunable-slip boundaries for coarse-grained simulations of fluid flow. *European Physical Journal E*, **2008**, 26, 115-22	1.5	44
89	Aqueous ionic liquids in comparison with standard co-solutes : Differences and common principles in their interaction with protein and DNA structures. *Biophysical Reviews*, **2018**, 10, 809-824	3.7	41
88	Aqueous ionic liquids and their influence on peptide conformations: denaturation and dehydration mechanisms. *Physical Chemistry Chemical Physics*, **2017**, 19, 20430-20440	3.6	41
87	Influence of the Compatible Solute Ectoine on the Local Water Structure: Implications for the Binding of the Protein G5P to DNA. *Journal of Physical Chemistry B*, **2015**, 119, 15212-20	3.4	39
86	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
85	The solvation and ion condensation properties for sulfonated polyelectrolytes in different solvents□ computational study. *New Journal of Physics*, **2014**, 16, 025001	2.9	35
84	Separation of chiral particles in micro- or nanofluidic channels. *Physical Review Letters*, **2012**, 108, 214504	7.4	35
83	Mesoscopic simulations of electroosmotic flow and electrophoresis in nanochannels. *Computer Physics Communications*, **2011**, 182, 1941-1944	4.2	35

82	Proton Dissociation of Sulfonated Polysulfones: Influence of Molecular Structure and Conformation. *Macromolecules*, **2015**, 48, 1134-1143	5.5	34
81	Atomistic insights into deep eutectic electrolytes: the influence of urea on the electrolyte salt LiTFSI in view of electrochemical applications. *Physical Chemistry Chemical Physics*, **2016**, 18, 28403-28408	3.6	33
80	Towards a Digital Bioprocess Replica: Computational Approaches in Biopharmaceutical Development and Manufacturing. *Trends in Biotechnology*, **2020**, 38, 1141-1153	15.1	32
79	Combined influence of ectoine and salt: spectroscopic and numerical evidence for compensating effects on aqueous solutions. *Physical Chemistry Chemical Physics*, **2016**, 18, 28398-28402	3.6	32
78	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
77	Stable conformations of a single stranded deprotonated DNA i-motif. *Journal of Physical Chemistry B*, **2011**, 115, 13788-95	3.4	31
76	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
75	The properties of residual water molecules in ionic liquids: a comparison between direct and inverse Kirkwood-Buff approaches. *Physical Chemistry Chemical Physics*, **2017**, 19, 18924-18937	3.6	28
74	Importance of varying permittivity on the conductivity of polyelectrolyte solutions. *Physical Review Letters*, **2015**, 115, 118301	7.4	28
73	Preferential Binding of Urea to Single-Stranded DNA Structures: A Molecular Dynamics Study. *Biophysical Journal*, **2018**, 114, 1551-1562	2.9	27
72	Polyelectrolyte electrophoresis in nanochannels: a dissipative particle dynamics simulation. *Journal of Physical Chemistry B*, **2010**, 114, 6266-72	3.4	27
71	Properties of Ion Complexes and Their Impact on Charge Transport in Organic Solvent-Based Electrolyte Solutions for Lithium Batteries: Insights from a Theoretical Perspective. *Batteries*, **2018**, 4, 62	5.7	27
70	Nudged-elastic band used to find reaction coordinates based on the free energy. *Journal of Chemical Physics*, **2014**, 140, 074109	3.9	26
69	Properties of Apolar Solutes in Alkyl Imidazolium-Based Ionic Liquids: The Importance of Local Interactions. *ChemPhysChem*, **2016**, 17, 387-94	3.2	26
68	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
67	Calculation of free energy landscapes: a histogram reweighted metadynamics approach. *Journal of Computational Chemistry*, **2011**, 32, 2084-96	3.5	25
66	Aqueous Mixtures of Room-Temperature Ionic Liquids: Entropy-Driven Accumulation of Water Molecules at Interfaces. *Journal of Physical Chemistry C*, **2019**, 123, 13795-13803	3.8	24
65	Properties of the polarizable MARTINI water model: A comparative study for aqueous electrolyte solutions. *Journal of Molecular Liquids*, **2015**, 212, 103-110	6	23

64	Validation of Trimethylamine-N-oxide (TMAO) Force Fields Based on Thermophysical Properties of Aqueous TMAO Solutions. *Journal of Physical Chemistry B*, **2017**, 121, 10674-10688	3.4	22
63	Preferential solvation and ion association properties in aqueous dimethyl sulfoxide solutions. *Physical Chemistry Chemical Physics*, **2016**, 18, 31312-31322	3.6	22
62	Deprotonation mechanism of a single-stranded DNA i-motif. *RSC Advances*, **2014**, 4, 17110-17113	3.7	22
61	Low concentrated hydroxyectoine solutions in presence of DPPC lipid bilayers: a computer simulation study. *Biophysical Chemistry*, **2013**, 180-181, 102-9	3.5	22
60	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
59	Influence of compatible solute ectoine on distinct DNA structures: thermodynamic insights into molecular binding mechanisms and destabilization effects. *Physical Chemistry Chemical Physics*, **2018**, 20, 25861-25874	3.6	20
58	Fluorinated Cyclic Phosphorus(III)-Based Electrolyte Additives for High Voltage Application in Lithium-Ion Batteries: Impact of Structure-Reactivity Relationships on CEI Formation and Cell Performance. *ACS Applied Materials & Interfaces*, **2019**, 11, 16605-16618	9.5	19
57	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
56	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
55	Theoretical and Computational Insight into Solvent and Specific Ion Effects for Polyelectrolytes: The Importance of Local Molecular Interactions. *Molecules*, **2020**, 25,	4.8	19
54	Enthalpic contributions to solvent-solute and solvent-ion interactions: Electronic perturbation as key to the understanding of molecular attraction. *Journal of Chemical Physics*, **2019**, 150, 174112	3.9	18
53	Aqueous Mixtures of Urea and Trimethylamine-N-oxide: Evidence for Kosmotropic or Chaotropic Behavior?. *Journal of Physical Chemistry B*, **2019**, 123, 4415-4424	3.4	18
52	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
51	A polarizable MARTINI model for monovalent ions in aqueous solution. *Journal of Chemical Physics*, **2018**, 149, 163319	3.9	17
50	Disentangling structural information from core-level excitation spectra. *Physical Review E*, **2017**, 96, 013319	2.4	17
49	Theoretical Insights into Specific Ion Effects and Strong-Weak Acid-Base Rules for Ions in Solution: Deriving the Law of Matching Solvent Affinities from First Principles. *ChemPhysChem*, **2020**, 21, 2605-2617	3.2	17
48	Unfolding of DNA by co-solutes: insights from KirkwoodBuff integrals and transfer free energies. *European Physical Journal: Special Topics*, **2019**, 227, 1665-1679	2.3	16
47	Mixtures of LiTFSI and urea: ideal thermodynamic behavior as key to the formation of deep eutectic solvents?. *Physical Chemistry Chemical Physics*, **2019**, 21, 12279-12287	3.6	15

46	LiPF6 Stabilizer and Transition-Metal Cation Scavenger: A Bifunctional Bipyridine-Based Ligand for Lithium-Ion Battery Application. *Chemistry of Materials*, **2019**, 31, 4025-4033	9.6	15
45	Lattice-Boltzmann simulations of the electrophoretic stretching of polyelectrolytes: the importance of hydrodynamic interactions. *Journal of Chemical Physics*, **2014**, 140, 164904	3.9	15
44	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
43	AFM-based force spectroscopy on polystyrene brushes: effect of brush thickness on protein adsorption. *Langmuir*, **2013**, 29, 1850-6	4	14
42	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
41	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
40	The Effect of Small Organic Cosolutes on Water Structure and Dynamics. *Journal of Chemical & Engineering Data*, **2020**, 65, 1197-1210	2.8	14
39	Specific Ion Effects and the Law of Matching Solvent Affinities: A Conceptual Density Functional Theory Approach. *Journal of Physical Chemistry B*, **2020**, 124, 2191-2197	3.4	13
38	Vibrational states of nano-confined water molecules in beryl investigated by first-principles calculations and optical experiments. *Physical Chemistry Chemical Physics*, **2017**, 19, 30740-30748	3.6	11
37	Layer-by-Layer Formation of Oligoelectrolyte Multilayers: A Combined Experimental and Computational Study. *Soft Materials*, **2014**, 12, S14-S21	1.7	11
36	Stretching of surface-tethered polymers in pressure-driven flow under confinement. *Soft Matter*, **2017**, 13, 6189-6196	3.6	11
35	Calculation of donor numbers: Computational estimates for the Lewis basicity of solvents. *Journal of Molecular Liquids*, **2021**, 322, 114506	6	11
34	Beneficial properties of solvents and ions for lithium ion and post-lithium ion batteries: Implications from charge transfer models. *Electrochimica Acta*, **2021**, 384, 138418	6.7	10
33	On the nature of ion-stabilized cytosine pairs in DNA i-motifs: The importance of charge transfer processes. *International Journal of Quantum Chemistry*, **2019**, 119, e25933	2.1	9
32	Systematic detection of hidden complexities in the unfolding mechanism of a cytosine-rich DNA strand. *Physica A: Statistical Mechanics and Its Applications*, **2014**, 394, 136-144	3.3	9
31	The stretching force on a tethered polymer in pressure-driven flow. *Journal of Chemical Physics*, **2017**, 147, 034902	3.9	9
30	Artificial neural networks for the prediction of solvation energies based on experimental and computational data. *Physical Chemistry Chemical Physics*, **2020**, 22, 24359-24364	3.6	8
29	Solvation in ionic liquid-water mixtures: A computational study. *Journal of Molecular Liquids*, **2019**, 292, 111273	6	7

28	Tetrahydrothiophene 1-oxide as highly effective co-solvent for propylene carbonate-based electrolytes. *Journal of Power Sources*, **2019**, 437, 226881	8.9	7
27	Non-Flammable Fluorinated Phosphorus(III)-Based Electrolytes for Advanced Lithium-Ion Battery Performance. *ChemElectroChem*, **2020**, 7, 1499-1508	4.3	6
26	Interactions of a DNA G-quadruplex with TMAO and urea: a molecular dynamics study on co-solute compensation mechanisms. *Physical Chemistry Chemical Physics*, **2021**, 23, 1254-1264	3.6	6
25	Conformation and Dynamics of Long-Chain End-Tethered Polymers in Microchannels. *Polymers*, **2019**, 11,	4.5	5
24	Mesoscopic Simulation Methods for Studying Flow and Transport in Electric Fields in Micro- and Nanochannels **2012**,		5
23	High Temperature Unfolding Simulations of a Single-stranded DNA i-Motif. *Current Physical Chemistry*, **2012**, 2, 115-123	0.5	5
22	Coat thickness dependent adsorption of hydrophobic molecules at polymer brushes. *Journal of Chemical Physics*, **2013**, 138, 044904	3.9	5
21	Complex transitions between dihydrate and anhydrate forms of ectoine unexpected behavior of a highly hygroscopic compatible solute in the solid state. *CrystEngComm*, **2020**, 22, 169-172	3.3	5
20	What Does Ectoine Do to DNA? A Molecular-Scale Picture of Compatible Solute-Biopolymer Interactions. *Journal of Physical Chemistry B*, **2020**, 124, 7999-8011	3.4	5
19	Raman Spectroscopic Signature of Ectoine Conformations in Bulk Solution and Crystalline State. *ChemPhysChem*, **2020**, 21, 1945-1950	3.2	4
18	Electronic Properties of Protein Destabilizers and Stabilizers: Implications for Preferential Binding and Exclusion Mechanisms. *Journal of Physical Chemistry B*, **2021**, 125, 11857-11868	3.4	4
17	Atomistic simulation of PDADMAC/PSS oligoelectrolyte multilayers: overall comparison of tri- and tetra-layer systems. *Soft Matter*, **2019**, 15, 9437-9451	3.6	4
16	Some Notes on the Thermodynamic Accuracy of Coarse-Grained Models. *Frontiers in Molecular Biosciences*, **2019**, 6, 87	5.6	4
15	Validation Is Not Verification: Precise Terminology and Scientific Methods in Bioprocess Modeling. *Trends in Biotechnology*, **2021**, 39, 1117-1119	15.1	3
14	Electric-field-induced stretching of surface-tethered polyelectrolytes in a microchannel. *Physical Review E*, **2017**, 96, 032503	2.4	2
13	Application of Tunable-Slip Boundary Conditions in Particle-Based Simulations **2015**, 19-30		2
12	Chapter 6:Free Energy Calculation Methods and Rare Event Sampling Techniques for Biomolecular Simulations. *RSC Theoretical and Computational Chemistry Series*, **2016**, 185-214	1.2	2
11	Generic and specific recurrent neural network models: Applications for large and small scale biopharmaceutical upstream processes. *Biotechnology Reports (Amsterdam, Netherlands)*, **2021**, 31, e00640	5.3	2

10	PDADMAC/PSS Oligoelectrolyte Multilayers: Internal Structure and Hydration Properties at Early Growth Stages from Atomistic Simulations. *Molecules*, **2020**, 25,	4.8	1
9	Atomistic Simulation of Oligoelectrolyte Multilayers Growth **2016**, 215-228		1
8	From the Atomistic to the Macromolecular Scale: Distinct Simulation Approaches for Polyelectrolyte Solutions **2018**, 1-15		1
7	Relaxation of surface-tethered polymers under moderate confinement. *Soft Matter*, **2018**, 14, 7926-7933	3.6	1
6	Energetic Arguments on the Microstructural Analysis in Ionic Liquids. *Advanced Theory and Simulations*, **2021**, 4, 2100114	3.5	0
5	Stabilization of DPPC lipid bilayers in the presence of co-solutes: molecular mechanisms and interaction patterns. *Physical Chemistry Chemical Physics*, **2021**, 23, 22936-22946	3.6	0
4	Holistic Process Models: A Bayesian Predictive Ensemble Method for Single and Coupled Unit Operation Models. *Processes*, **2022**, 10, 662	2.9	0
3	Force Field Optimization for Ionic Liquids: FFOIL **2016**, 101-117		
2	Mesoscopic Simulations of Polyelectrolyte Electrophoresis in Nanochannels **2011**, 53-67		
1	From the Atomistic to the Macromolecular Scale: Distinct Simulation Approaches for Polyelectrolyte Solutions **2020**, 1381-1395		