Othmar Steinhauser

List of Publications by Year
in descending order

106 papers	4,537 citations	100601 38 h-index	124990 64 g-index
109 all docs	109 docs citations	109 times ranked	3217 citing authors

#	Article	IF	Citations
1	Emulating proton transfer reactions in the pseudo-protic ionic liquid 1-methylimidazolium acetate. Physical Chemistry Chemical Physics, 2022, 24, 9277-9285.	1.3	8
2	The Intermolecular NOE Depends on Isotope Selection: Short Range vs Long Range Behavior. Journal of Physical Chemistry Letters, 2021, 12, 8658-8663.	2.1	6
3	The proteinâ€“water nuclear Overhauser effect (NOE) as an indirect microscope for molecular surface mapping of interaction patterns. Physical Chemistry Chemical Physics, 2020, 22, 212-222.	1.3	6
4	Dielectric spectroscopy and time dependent Stokes shift: two faces of the same coin?. Physical Chemistry Chemical Physics, 2020, 22, 18388-18399.	1.3	1
5	Understanding the Nature of Nuclear Magnetic Resonance Relaxation by Means of Fast-Field-Cycling Relaxometry and Molecular Dynamics Simulationsâ€”The Validity of Relaxation Models. Journal of Physical Chemistry Letters, 2020, 11, 2165-2170.	2.1	21
6	The nuclear Overhauser Effect (NOE) as a tool to study macromolecular confinement: Elucidation and disentangling of crowding and encapsulation effects. Journal of Chemical Physics, 2020, 152, 024120.	1.2	1
7	Hydration dynamics of proteins in reverse micelles probed by¹H-NOESY/¹H-ROESY NMR and¹⁷O-nuclear quadrupole resonance (NQR). Physical Chemistry Chemical Physics, 2019, 21, 14571-14582.	1.3	4
8	Computational spectroscopy of trehalose, sucrose, maltose, and glucose: A comprehensive study of TDSS, NQR, NOE, and DRS. Journal of Chemical Physics, 2019, 150, 175102.	1.2	10
9	Towards capturing cellular complexity: combining encapsulation and macromolecular crowding in a reverse micelle. Physical Chemistry Chemical Physics, 2019, 21, 8108-8120.	1.3	7
10	Changes in protein hydration dynamics by encapsulation or crowding of ubiquitin: strong correlation between time-dependent Stokes shift and intermolecular nuclear Overhauser effect. RSC Advances, 2019, 9, 36982-36993.	1.7	5
11	Micellar confinement disrupts collective structure and accelerates collective dynamics of encapsulated water. Physical Chemistry Chemical Physics, 2018, 20, 11454-11469.	1.3	19
12	Molecular dynamics simulation of aqueous 1â€˜dodecylâ€˜3â€˜methylimidazolium chloride: Emerging micelles. Journal of Molecular Liquids, 2018, 272, 766-777.	2.3	10
13	A shell-resolved analysis of preferential solvation of coffee ingredients in aqueous mixtures of the ionic liquid 1-ethyl-3-methylimidazolium acetate. Journal of Chemical Physics, 2018, 148, 193819.	1.2	17
14	Langevin behavior of the dielectric decrement in ionic liquid water mixtures. Physical Chemistry Chemical Physics, 2018, 20, 15106-15117.	1.3	19
15	Macromolecular crowding and the importance of proper hydration for the structure and dynamics of protein solutions. Physical Chemistry Chemical Physics, 2018, 20, 19581-19594.	1.3	11
16	Revival of collective water structure and dynamics in reverse micelles brought about by protein encapsulation. Physical Chemistry Chemical Physics, 2018, 20, 22932-22945.	1.3	10
17	Towards a complete characterization of the Î´-dispersion in dielectric spectroscopy of proteinâ€“water systems. Physical Chemistry Chemical Physics, 2017, 19, 26980-26985.	1.3	23
18	Revival of the Intermolecular Nuclear Overhauser Effect for Mapping Local Protein Hydration Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 3421-3426.	2.1	19

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19	A computational component analysis of dielectric relaxation and THz spectra of water/AOT reverse micelles with different water loading. Journal of Chemical Physics, 2016, 145, 214702.	1.2	13
20	Rotational dynamics of water molecules near biological surfaces with implications for nuclear quadrupole relaxation. Physical Chemistry Chemical Physics, 2016, 18, 24620-24630.	1.3	28
21	Combining non-equilibrium simulations and coarse-grained modelling allows for a fine-grained decomposition of solvation dynamics. Physical Chemistry Chemical Physics, 2016, 18, 30954-30960.	1.3	5
22	Charged, dipolar soft matter systems from a combined microscopicâ€“mesoscopic viewpoint. Journal of Physics Condensed Matter, 2016, 28, 344008.	0.7	2
23	Dielectric depolarisation and concerted collective dynamics in AOT reverse micelles with and without ubiquitin. Physical Chemistry Chemical Physics, 2016, 18, 3606-3617.	1.3	17
24	Additive polarizabilities in ionic liquids. Physical Chemistry Chemical Physics, 2016, 18, 1665-1670.	1.3	37
25	Comparing induced point-dipoles and Drude oscillators. Physical Chemistry Chemical Physics, 2015, 17, 14297-14306.	1.3	36
26	Orientational Alignment of Amyloidogenic Proteins in Pre-Aggregated Solutions. Physical Review Letters, 2015, 114, 128101.	2.9	11
27	The intermolecular NOE is strongly influenced by dynamics. Physical Chemistry Chemical Physics, 2015, 17, 8509-8517.	1.3	27
28	Pair dynamics and the intermolecular nuclear Overhauser effect (NOE) in liquids analysed by simulation and model theories: Application to an ionic liquid. Journal of Chemical Physics, 2014, 140, 184503.	1.2	29
29	On the collective network of ionic liquid/water mixtures. IV. Kinetic and rotational depolarization. Journal of Chemical Physics, 2014, 140, 204505.	1.2	13
30	Transport and dielectric properties of water and the influence of coarse-graining: Comparing BMW, SPC/E, and TIP3P models. Journal of Chemical Physics, 2014, 140, 064107.	1.2	55
31	Dielectric spectra of ionic liquids and their conversion to solvation dynamics: a detailed computational analysis of polarizable systems. Physical Chemistry Chemical Physics, 2014, 16, 10999-11009.	1.3	19
32	From Shortâ€Range to Longâ€Range Intermolecular NOEs in Ionic Liquids: Frequency Does Matter. Angewandte Chemie - International Edition, 2013, 52, 9242-9246.	7.2	36
33	Polarization effects on the solvation dynamics of coumarin C153 in ionic liquids: Components and their cross-correlations. Journal of Chemical Physics, 2013, 138, 204504.	1.2	30
34	The effect of Thole functions on the simulation of ionic liquids with point induced dipoles at various densities. Journal of Chemical Physics, 2013, 138, 204119.	1.2	18
35	Hydrated Ionic Liquids with and without Solute: The Influence of Water Content and Protein Solutes. Journal of Chemical Theory and Computation, 2012, 8, 3911-3928.	2.3	47
36	Computational studies of ionic liquids: Size does matter and time too. Journal of Chemical Physics, 2012, 137, 094501.	1.2	64

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37	Solvation studies of a zinc finger protein in hydrated ionic liquids. Physical Chemistry Chemical Physics, 2011, 13, 6955.	1.3	45
38	On the influence of hydrated ionic liquids on the dynamical structure of model proteins: a computational study. Physical Chemistry Chemical Physics, 2011, 13, 17994.	1.3	34
39	The influence of polarizability on the dielectric spectrum of the ionic liquid 1-ethyl-3-methylimidazolium triflate. Physical Chemistry Chemical Physics, 2011, 13, 12240.	1.3	47
40	Simulating polarizable molecular ionic liquids with Drude oscillators. Journal of Chemical Physics, 2010, 133, 154511.	1.2	98
41	Global and local Voronoi analysis of solvation shells of proteins. Journal of Chemical Physics, 2010, 133, 084108.	1.2	18
42	Using fit functions in computational dielectric spectroscopy. Journal of Chemical Physics, 2010, 132, 244109.	1.2	54
43	Relaxation of Voronoi shells in hydrated molecular ionic liquids. Journal of Chemical Physics, 2009, 131, 174509.	1.2	33
44	On the collective network of ionic liquid/water mixtures. III. Structural analysis of ionic liquids on the basis of Voronoi decomposition. Journal of Chemical Physics, 2009, 130, 194503.	1.2	50
45	On the dielectric conductivity of molecular ionic liquids. Journal of Chemical Physics, 2009, 131, 114504.	1.2	58
46	Analysis of key parameters for molecular dynamics of pMHC molecules. Molecular Simulation, 2008, 34, 781-793.	0.9	37
47	On the computation and contribution of conductivity in molecular ionic liquids. Journal of Chemical Physics, 2008, 128, 134501.	1.2	117
48	The influence of electrostatic forces on the structure and dynamics of molecular ionic liquids. Journal of Chemical Physics, 2008, 128, 224503.	1.2	49
49	On the collective network of ionic liquid/water mixtures. II. Decomposition and interpretation of dielectric spectra. Journal of Chemical Physics, 2008, 129, 184501.	1.2	95
50	Grid Services for Parallel Molecular Dynamics with NAMD and CHARMM. Lecture Notes in Computer Science, 2008, , 1036-1051.	1.0	1
51	Impact of anisotropy on the structure and dynamics of ionic liquids: A computational study of 1-butyl-3-methyl-imidazolium trifluoroacetate. Journal of Chemical Physics, 2007, 127, 044505.	1.2	49
52	On the collective network of ionic liquid/water mixtures. I. Orientational structure. Journal of Chemical Physics, 2007, 127, 234503.	1.2	120
53	Collective rotational dynamics in ionic liquids: A computational and experimental study of 1-butyl-3-methyl-imidazolium tetrafluoroborate. Journal of Chemical Physics, 2007, 126, 084511.	1.2	93
54	Simulation studies of ionic liquids: Orientational correlations and static dielectric properties. Journal of Chemical Physics, 2006, 125, 244506.	1.2	99

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55	Simulation studies of the protein-water interface. II. Properties at the mesoscopic resolution. Journal of Chemical Physics, 2006, 124, 234908.	1.2	39
56	Simulation studies of the protein-water interface. I. Properties at the molecular resolution. Journal of Chemical Physics, 2006, 124, 234907.	1.2	75
57	Rapid Assessment of Protein Structural Stability and Fold Validation via NMR. Methods in Enzymology, 2005, 394, 142-175.	0.4	17
58	A molecular dynamics study of the dielectric properties of aqueous solutions of alanine and alanine dipeptide. Journal of Chemical Physics, 2004, 120, 3333-3347.	1.2	34
59	Comments on â€œAnomalous Dielectric Relaxation of Aqueous Protein Solutionsâ€•by Nilashis Nandi and Biman Bagchi (J. Phys. Chem. A1998,102, 8217). Journal of Physical Chemistry A, 2001, 105, 5507-5508.	1.1	3
60	Dielectric spectroscopy in aqueous solutions of oligosaccharides: Experiment meets simulation. Journal of Chemical Physics, 2001, 115, 1463-1472.	1.2	52
61	The dielectric self-consistent field method. II. Application to the study of finite range effects. Journal of Chemical Physics, 2001, 115, 10793-10807.	1.2	24
62	The dielectric self-consistent field method. I. Highways, byways, and illustrative results. Journal of Chemical Physics, 2001, 115, 10780-10792.	1.2	18
63	Making use of Connollyâ€™s molecular surface program in the isodensity adapted polarizable continuum model. Journal of Chemical Physics, 2001, 115, 10636-10646.	1.2	3
64	Studying the Dielectric Properties of a Protein Solution by Computer Simulation. Journal of Physical Chemistry B, 2000, 104, 8743-8752.	1.2	74
65	Performance Analysis, PVM and MPI Implementation of a DSCF Hartree Fock Program. Journal of Computing and Information Technology, 2000, 8, 19.	0.2	4
66	Towards a better description and understanding of biomolecular solvation. Biophysical Chemistry, 1999, 78, 43-68.	1.5	43
67	Rationalizing the effects of modified electrostatic interactions in computer simulations: The dielectric self-consistent field method. Journal of Chemical Physics, 1999, 111, 8271-8274.	1.2	22
68	A molecular dynamics simulation study of the unfolding of barnase induced by reaction field perturbation. Physical Chemistry Chemical Physics, 1999, 1, 4355-4370.	1.3	1
69	X-ray structure and conformational dynamics of the HIV-1 protease in complex with the inhibitor SDZ283-910: agreement of time-resolved spectroscopy and molecular dynamics simulations 1 1Edited by R. Huber. Journal of Molecular Biology, 1999, 286, 1147-1159.	2.0	24
70	Performance Analysis and Derived Parallelization Strategy for a SCF Program at the Hartree Fock Level. Lecture Notes in Computer Science, 1999, , 163-172.	1.0	7
71	Rationalization of the dielectric properties of common three-site water models in terms of their force field parameters. Journal of Chemical Physics, 1998, 109, 4927-4937.	1.2	128
72	The frequency-dependent conductivity of a saturated solution of ZnBr2 in water: A molecular dynamics simulation. Journal of Chemical Physics, 1997, 107, 3135-3143.	1.2	18

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73	Calculation of the dielectric properties of a protein and its solvent: theory and a case study. Journal of Molecular Biology, 1997, 270, 520-534.	2.0	128
74	The Temperature-Dependence of Hydrophobic Association in Water. Pair versus Bulk Hydrophobic Interactions. Journal of the American Chemical Society, 1997, 119, 4206-4213.	6.6	94
75	Presumed versus real artifacts of the Ewald summation technique: The importance of dielectric boundary conditions. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1997, 101, 1019-1029.	0.9	46
76	Parallel biomolecular simulation: Theory, algorithms and implementation. Simulation Modelling Practice and Theory, 1997, 5, 573-603.	0.4	1
77	The influence of a protein on water dynamics in its vicinity investigated by molecular dynamics simulation. , 1996, 25, 366-378.		102
78	The influence of temperature on pairwise hydrophobic interactions of methaneâ€like particles: A molecular dynamics study of free energy. Journal of Chemical Physics, 1996, 104, 286-295.	1.2	93
79	NMR Cross-relaxation Investigated by Molecular Dynamics Simulation: A Case Study of Ubiquitin in Solution. Journal of Molecular Biology, 1995, 249, 604-624.	2.0	23
80	Influence of Molecular Motion on the Accuracy of NMR-Derived Distances. A Molecular Dynamics Study of Two Solvated Model Peptides. Journal of the American Chemical Society, 1994, 116, 4006-4018.	6.6	23
81	Cutoff size does strongly influence molecular dynamics results on solvated polypeptides. Biochemistry, 1992, 31, 5856-5860.	1.2	217
82	Taming cut-off induced artifacts in molecular dynamics studies of solvated polypeptides. Journal of Molecular Biology, 1992, 228, 909-923.	2.0	87
83	Parallel molecular dynamics of biomolecules. Parallel Computing, 1992, 18, 557-573.	1.3	26
84	Molecular dynamics studies of solvated polypeptides: Why the cut-off scheme does not work. Chemical Physics, 1992, 168, 75-89.	0.9	117
85	The effect of density variation on the structure of liquid hydrogen chloride. A Monte Carlo study. Journal of Chemical Physics, 1990, 93, 2357-2363.	1.2	19
86	Symmetry reduction of the RISM equation. Chemical Physics Letters, 1985, 116, 465-470.	1.2	15
87	Computer simulation and the dielectric constant of polarizable polar systems. Chemical Physics Letters, 1984, 106, 563-569.	1.2	112
88	Consistent calculation of the static and frequency-dependent dielectric constant in computer simulations. Molecular Physics, 1984, 52, 97-113.	0.8	214
89	On the calculation of the dielectric constant using the Ewald-Kornfeld tensor. Chemical Physics Letters, 1983, 95, 417-422.	1.2	113
90	On the calculation of the frequency-dependent dielectric constant in computer simulations. Chemical Physics Letters, 1983, 102, 508-513.	1.2	98

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91	On the dielectric theory and computer simulation of water. Chemical Physics, 1983, 79, 465-482.	0.9	24
92	On the Orientational Structure and Dielectric Properties of Water. A Comparison of ST2 and MCY Potential. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1983, 87, 128-142.	0.9	25
93	Computer simulation of polar liquids the influence of molecular shape. Molecular Physics, 1982, 46, 827-837.	0.8	12
94	Reaction field simulation of water. Molecular Physics, 1982, 45, 335-348.	0.8	195
95	On the structure and dynamics of liquid benzene. Chemical Physics, 1982, 73, 155-167.	0.9	50
96	Pair correlation functions of liquid CS2. A comparison between statistical-mechanical theories and computer simulation. Chemical Physics Letters, 1981, 80, 89-93.	1.2	14
97	Single particle dynamics of liquid carbon disulfide. Chemical Physics Letters, 1981, 82, 153-157.	1.2	16
98	Molecular pair correlation function of liquid acetonitrile derived from perturbation theory with a computer-generated reference function. Chemical Physics Letters, 1981, 78, 555-559.	1.2	22
99	The influence of boundary conditions used in machine simulations on the structure of polar systems. Molecular Physics, 1980, 39, 437-454.	0.8	111
100	Structure and dynamics of liquid carbon tetrachloride.. Molecular Physics, 1980, 40, 115-128.	0.8	63
101	Structure of liquid carbon disulphide: a molecular dynamics study. Molecular Physics, 1979, 37, 1921-1939.	0.8	50
102	Solvation of large dipoles. Molecular Physics, 1979, 37, 1725-1743.	0.8	10
103	Solvation of large dipoles. Molecular Physics, 1978, 35, 841-855.	0.8	21
104	Multipole expansion of diatomic overlap. Theoretica Chimica Acta, 1977, 45, 147-156.	0.9	2
105	Multipole expansion of diatomic overlap. Theoretica Chimica Acta, 1977, 46, 157-164.	0.9	1
106	Collectivity in ionic liquids: A temperature-dependent, polarizable molecular dynamics study.. Physical Chemistry Chemical Physics, 0, , .	1.3	3