Othmar Steinhauser

List of Publications by Year in Descending Order

106 papers	4,131 citations	38 h-index	61 g-index
109 ext. papers	4,348 ext. citations	3.8 avg, IF	5.46 L-index

#	Paper	IF	Citations
106	The Intermolecular NOE Depends on Isotope Selection: Short Range vs Long Range Behavior. *Journal of Physical Chemistry Letters*, **2021**, 12, 8658-8663	6.4	1
105	Understanding the Nature of Nuclear Magnetic Resonance Relaxation by Means of Fast-Field-Cycling Relaxometry and Molecular Dynamics Simulations-The Validity of Relaxation Models. *Journal of Physical Chemistry Letters*, **2020**, 11, 2165-2170	6.4	12
104	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	3.9	0
103	Dielectric spectroscopy and time dependent Stokes shift: two faces of the same coin?. *Physical Chemistry Chemical Physics*, **2020**, 22, 18388-18399	3.6	1
102	Hydration dynamics of proteins in reverse micelles probed by H-NOESY/H-ROESY NMR and O-nuclear quadrupole resonance (NQR). *Physical Chemistry Chemical Physics*, **2019**, 21, 14571-14582	3.6	3
101	Computational spectroscopy of trehalose, sucrose, maltose, and glucose: A comprehensive study of TDSS, NQR, NOE, and DRS. *Journal of Chemical Physics*, **2019**, 150, 175102	3.9	5
100	Towards capturing cellular complexity: combining encapsulation and macromolecular crowding in a reverse micelle. *Physical Chemistry Chemical Physics*, **2019**, 21, 8108-8120	3.6	6
99	The protein-water nuclear Overhauser effect (NOE) as an indirect microscope for molecular surface mapping of interaction patterns. *Physical Chemistry Chemical Physics*, **2019**, 22, 212-222	3.6	2
98	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	3.7	4
97	Micellar confinement disrupts collective structure and accelerates collective dynamics of encapsulated water. *Physical Chemistry Chemical Physics*, **2018**, 20, 11454-11469	3.6	16
96	Macromolecular crowding and the importance of proper hydration for the structure and dynamics of protein solutions. *Physical Chemistry Chemical Physics*, **2018**, 20, 19581-19594	3.6	9
95	Revival of collective water structure and dynamics in reverse micelles brought about by protein encapsulation. *Physical Chemistry Chemical Physics*, **2018**, 20, 22932-22945	3.6	10
94	Molecular dynamics simulation of aqueous 1-dodecyl-3-methylimidazolium chloride: Emerging micelles. *Journal of Molecular Liquids*, **2018**, 272, 766-777	6	7
93	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	3.9	13
92	Langevin behavior of the dielectric decrement in ionic liquid water mixtures. *Physical Chemistry Chemical Physics*, **2018**, 20, 15106-15117	3.6	13
91	Towards a complete characterization of the δ-dispersion in dielectric spectroscopy of protein-water systems. *Physical Chemistry Chemical Physics*, **2017**, 19, 26980-26985	3.6	17
90	Revival of the Intermolecular Nuclear Overhauser Effect for Mapping Local Protein Hydration Dynamics. *Journal of Physical Chemistry Letters*, **2017**, 8, 3421-3426	6.4	17

89	Rotational dynamics of water molecules near biological surfaces with implications for nuclear quadrupole relaxation. *Physical Chemistry Chemical Physics*, **2016**, 18, 24620-30	3.6	23
88	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	3.6	5
87	Charged, dipolar soft matter systems from a combined microscopic-mesoscopic viewpoint. *Journal of Physics Condensed Matter*, **2016**, 28, 344008	1.8	2
86	Dielectric depolarisation and concerted collective dynamics in AOT reverse micelles with and without ubiquitin. *Physical Chemistry Chemical Physics*, **2016**, 18, 3606-17	3.6	16
85	Additive polarizabilities in ionic liquids. *Physical Chemistry Chemical Physics*, **2016**, 18, 1665-70	3.6	27
84	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	3.9	11
83	Orientational alignment of amyloidogenic proteins in pre-aggregated solutions. *Physical Review Letters*, **2015**, 114, 128101	7.4	10
82	The intermolecular NOE is strongly influenced by dynamics. *Physical Chemistry Chemical Physics*, **2015**, 17, 8509-17	3.6	24
81	Comparing induced point-dipoles and Drude oscillators. *Physical Chemistry Chemical Physics*, **2015**, 17, 14297-306	3.6	27
80	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	3.9	45
79	Dielectric spectra of ionic liquids and their conversion to solvation dynamics: a detailed computational analysis of polarizable systems. *Physical Chemistry Chemical Physics*, **2014**, 16, 10999-1009	3.6	18
78	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	3.9	28
77	On the collective network of ionic liquid/water mixtures. IV. Kinetic and rotational depolarization. *Journal of Chemical Physics*, **2014**, 140, 204505	3.9	11
76	From short-range to long-range intermolecular NOEs in ionic liquids: frequency does matter. *Angewandte Chemie - International Edition*, **2013**, 52, 9242-6	16.4	32
75	From Short-Range to Long-Range Intermolecular NOEs in Ionic Liquids: Frequency Does Matter. *Angewandte Chemie*, **2013**, 125, 9412-9416	3.6	18
74	Polarization effects on the solvation dynamics of coumarin C153 in ionic liquids: components and their cross-correlations. *Journal of Chemical Physics*, **2013**, 138, 204504	3.9	27
73	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	3.9	12
72	Titelbild: From Short-Range to Long-Range Intermolecular NOEs in Ionic Liquids: Frequency Does Matter (Angew. Chem. 35/2013). *Angewandte Chemie*, **2013**, 125, 9221-9221	3.6	

71	Hydrated Ionic Liquids with and without Solute: The Influence of Water Content and Protein Solutes. *Journal of Chemical Theory and Computation*, **2012**, 8, 3911-28	6.4	43
70	Computational studies of ionic liquids: size does matter and time too. *Journal of Chemical Physics*, **2012**, 137, 094501	3.9	58
69	On the influence of hydrated ionic liquids on the dynamical structure of model proteins: a computational study. *Physical Chemistry Chemical Physics*, **2011**, 13, 17994-8004	3.6	32
68	The influence of polarizability on the dielectric spectrum of the ionic liquid 1-ethyl-3-methylimidazolium triflate. *Physical Chemistry Chemical Physics*, **2011**, 13, 12240-8	3.6	39
67	Solvation studies of a zinc finger protein in hydrated ionic liquids. *Physical Chemistry Chemical Physics*, **2011**, 13, 6955-69	3.6	43
66	Simulating polarizable molecular ionic liquids with Drude oscillators. *Journal of Chemical Physics*, **2010**, 133, 154511	3.9	77
65	Global and local Voronoi analysis of solvation shells of proteins. *Journal of Chemical Physics*, **2010**, 133, 084108	3.9	16
64	Using fit functions in computational dielectric spectroscopy. *Journal of Chemical Physics*, **2010**, 132, 244109	3.9	45
63	Computational Dielectric Spectroscopy of Charged, Dipolar Systems **2010**, 279-321		4
62	Relaxation of Voronoi shells in hydrated molecular ionic liquids. *Journal of Chemical Physics*, **2009**, 131, 174509	3.9	33
61	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	3.9	46
60	On the dielectric conductivity of molecular ionic liquids. *Journal of Chemical Physics*, **2009**, 131, 114504	3.9	53
59	Analysis of key parameters for molecular dynamics of pMHC molecules. *Molecular Simulation*, **2008**, 34, 781-793	2	34
58	On the computation and contribution of conductivity in molecular ionic liquids. *Journal of Chemical Physics*, **2008**, 128, 134501	3.9	100
57	The influence of electrostatic forces on the structure and dynamics of molecular ionic liquids. *Journal of Chemical Physics*, **2008**, 128, 224503	3.9	48
56	On the collective network of ionic liquid/water mixtures. II. Decomposition and interpretation of dielectric spectra. *Journal of Chemical Physics*, **2008**, 129, 184501	3.9	83
55	Grid Services for Parallel Molecular Dynamics with NAMD and CHARMM. *Lecture Notes in Computer Science*, **2008**, 1036-1051	0.9	0
54	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	3.9	47

53	On the collective network of ionic liquid/water mixtures. I. Orientational structure. *Journal of Chemical Physics*, **2007**, 127, 234503	3.9	114
52	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	3.9	87
51	Simulation studies of the protein-water interface. II. Properties at the mesoscopic resolution. *Journal of Chemical Physics*, **2006**, 124, 234908	3.9	36
50	Simulation studies of the protein-water interface. I. Properties at the molecular resolution. *Journal of Chemical Physics*, **2006**, 124, 234907	3.9	66
49	Simulation studies of ionic liquids: orientational correlations and static dielectric properties. *Journal of Chemical Physics*, **2006**, 125, 244506	3.9	91
48	Rapid assessment of protein structural stability and fold validation via NMR. *Methods in Enzymology* , **2005**, 394, 142-75	1.7	16
47	A molecular dynamics study of the dielectric properties of aqueous solutions of alanine and alanine dipeptide. *Journal of Chemical Physics*, **2004**, 120, 3333-47	3.9	32
46	Dielectric spectroscopy in aqueous solutions of oligosaccharides: Experiment meets simulation. *Journal of Chemical Physics*, **2001**, 115, 1463-1472	3.9	49
45	The dielectric self-consistent field method. II. Application to the study of finite range effects. *Journal of Chemical Physics*, **2001**, 115, 10793-10807	3.9	23
44	The dielectric self-consistent field method. I. Highways, byways, and illustrative results. *Journal of Chemical Physics*, **2001**, 115, 10780-10792	3.9	16
43	Making use of Connolly molecular surface program in the isodensity adapted polarizable continuum model. *Journal of Chemical Physics*, **2001**, 115, 10636-10646	3.9	3
42	Comments on Anomalous Dielectric Relaxation of Aqueous Protein Solutions by Nilashis Nandi and Biman Bagchi (J. Phys. Chem. A 1998, 102, 8217). *Journal of Physical Chemistry A*, **2001**, 105, 5507-5508	2.8	3
41	Studying the Dielectric Properties of a Protein Solution by Computer Simulation. *Journal of Physical Chemistry B*, **2000**, 104, 8743-8752	3.4	61
40	Performance Analysis, PVM and MPI Implementation of a DSCF Hartree Fock Program. *Journal of Computing and Information Technology*, **2000**, 8, 19	0.4	4
39	Towards a better description and understanding of biomolecular solvation. *Biophysical Chemistry*, **1999**, 78, 43-68	3.5	40
38	Rationalizing the effects of modified electrostatic interactions in computer simulations: The dielectric self-consistent field method. *Journal of Chemical Physics*, **1999**, 111, 8271-8274	3.9	21
37	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. *Journal of Molecular Biology*, **1999**, 286, 1147-59	6.5	24
36	Performance Analysis and Derived Parallelization Strategy for a SCF Program at the Hartree Fock Level. *Lecture Notes in Computer Science*, **1999**, 163-172	0.9	6

35	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	3.9	125
34	The frequency-dependent conductivity of a saturated solution of ZnBr2 in water: A molecular dynamics simulation. *Journal of Chemical Physics*, **1997**, 107, 3135-3143	3.9	15
33	Calculation of the dielectric properties of a protein and its solvent: theory and a case study. *Journal of Molecular Biology*, **1997**, 270, 520-34	6.5	111
32	The Temperature-Dependence of Hydrophobic Association in Water. Pair versus Bulk Hydrophobic Interactions. *Journal of the American Chemical Society*, **1997**, 119, 4206-4213	16.4	86
31	Presumed versus real artifacts of the Ewald summation technique: The importance of dielectric boundary conditions. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1997**, 101, 1019-1029		46
30	Parallel biomolecular simulation: Theory, algorithms and implementation. *Simulation Modelling Practice and Theory*, **1997**, 5, 573-603		1
29	The influence of a protein on water dynamics in its vicinity investigated by molecular dynamics simulation. *Proteins: Structure, Function and Bioinformatics*, **1996**, 25, 366-78	4.2	98
28	The influence of temperature on pairwise hydrophobic interactions of methane-like particles: A molecular dynamics study of free energy. *Journal of Chemical Physics*, **1996**, 104, 286-295	3.9	86
27	NMR cross-relaxation investigated by molecular dynamics simulation: a case study of ubiquitin in solution. *Journal of Molecular Biology*, **1995**, 249, 604-24	6.5	23
26	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	16.4	20
25	Cutoff size does strongly influence molecular dynamics results on solvated polypeptides. *Biochemistry*, **1992**, 31, 5856-60	3.2	207
24	Taming cut-off induced artifacts in molecular dynamics studies of solvated polypeptides. The reaction field method. *Journal of Molecular Biology*, **1992**, 228, 909-23	6.5	82
23	Parallel molecular dynamics of biomolecules. *Parallel Computing*, **1992**, 18, 557-573	1	21
22	Molecular dynamics studies of solvated polypeptides: Why the cut-off scheme does not work. *Chemical Physics*, **1992**, 168, 75-89	2.3	116
21	The effect of density variation on the structure of liquid hydrogen chloride. A Monte Carlo study. *Journal of Chemical Physics*, **1990**, 93, 2357-2363	3.9	19
20	Symmetry reduction of the RISM equation. *Chemical Physics Letters*, **1985**, 116, 465-470	2.5	14
19	Computer simulation and the dielectric constant of polarizable polar systems. *Chemical Physics Letters*, **1984**, 106, 563-569	2.5	100
18	Consistent calculation of the static and frequency-dependent dielectric constant in computer simulations. *Molecular Physics*, **1984**, 52, 97-113	1.7	201

17	On the calculation of the dielectric constant using the Ewald-Kornfeld tensor. *Chemical Physics Letters*, **1983**, 95, 417-422	2.5	112
16	On the calculation of the frequency-dependent dielectric constant in computer simulations. *Chemical Physics Letters*, **1983**, 102, 508-513	2.5	89
15	On the dielectric theory and computer simulation of water. *Chemical Physics*, **1983**, 79, 465-482	2.3	23
14	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		23
13	Computer simulation of polar liquids the influence of molecular shape. *Molecular Physics*, **1982**, 46, 827-837	1.7	12
12	Reaction field simulation of water. *Molecular Physics*, **1982**, 45, 335-348	1.7	189
11	On the structure and dynamics of liquid benzene. *Chemical Physics*, **1982**, 73, 155-167	2.3	47
10	Pair correlation functions of liquid CS2. A comparison between statistical-mechanical theories and computer simulation. *Chemical Physics Letters*, **1981**, 80, 89-93	2.5	13
9	Single particle dynamics of liquid carbon disulfide. *Chemical Physics Letters*, **1981**, 82, 153-157	2.5	16
8	Molecular pair correlation function of liquid acetonitrile derived from perturbation theory with a computer-generated reference function. *Chemical Physics Letters*, **1981**, 78, 555-559	2.5	20
7	The influence of boundary conditions used in machine simulations on the structure of polar systems. *Molecular Physics*, **1980**, 39, 437-454	1.7	107
6	Structure and dynamics of liquid carbon tetrachloride.. *Molecular Physics*, **1980**, 40, 115-128	1.7	62
5	Solvation of large dipoles. *Molecular Physics*, **1979**, 37, 1725-1743	1.7	10
4	Structure of liquid carbon disulphide: a molecular dynamics study. *Molecular Physics*, **1979**, 37, 1921-1939	1.7	49
3	Solvation of large dipoles. *Molecular Physics*, **1978**, 35, 841-855	1.7	19
2	Multipole expansion of diatomic overlap. *Theoretica Chimica Acta*, **1977**, 45, 147-156		2
1	Multipole expansion of diatomic overlap. *Theoretica Chimica Acta*, **1977**, 46, 157-164		1