Dietmar Paschek

List of Publications by Year in Descending Order

101 papers	4,412 citations	38 h-index	64 g-index
116 ext. papers	4,709 ext. citations	5.1 avg, IF	5.86 L-index

#	Paper	IF	Citations
101	Why Do Liquids Mix? The Mixing of Protic Ionic Liquids Sharing the Same Cation Is Apparently Driven by Enthalpy, Not Entropy.. *Journal of Physical Chemistry Letters*, **2022**, 3556-3561	6.4	0
100	Kinetics of Hydrogen Bonding between Ions with Opposite and Like Charges in Hydroxyl-Functionalized Ionic Liquids. *Journal of Physical Chemistry B*, **2021**, 125, 281-286	3.4	5
99	Balance Between Contact and Solvent-Separated Ion Pairs in Mixtures of the Protic Ionic Liquid [EtNH][MeSO] with Water Controlled by Water Content and Temperature. *Journal of Physical Chemistry B*, **2021**, 125, 4476-4488	3.4	3
98	Structural similarity of an ionic liquid and the mixture of the neutral molecules. *Journal of Molecular Liquids*, **2021**, 329, 115589	6	4
97	Hydrogen Bonds between Ions of Opposite and Like Charge in Hydroxyl-Functionalized Ionic Liquids: an Exhaustive Examination of the Interplay between Global and Local Motions and Intermolecular Hydrogen Bond Lifetimes and Kinetics. *Journal of Physical Chemistry B*, **2021**, 125, 5132-5144	3.4	3
96	An exact a posteriori correction for hydrogen bond population correlation functions and other reversible geminate recombinations obtained from simulations with periodic boundary conditions. Liquid water as a test case. *Journal of Chemical Physics*, **2021**, 154, 214501	3.9	
95	Quasi-Universal Solubility Behavior of Light Gases in Imidazolium-Based Ionic Liquids with Varying Anions: A Molecular Dynamics Simulation Study. *Journal of Physical Chemistry B*, **2021**, 125, 1647-1659	3.4	4
94	Counting cations involved in cationic clusters of hydroxy-functionalized ionic liquids by means of infrared and solid-state NMR spectroscopy. *Physical Chemistry Chemical Physics*, **2020**, 22, 6861-6867	3.6	9
93	Comparing the void space and long-range structure of an ionic liquid with a neutral mixture of similar sized molecules. *Journal of Molecular Liquids*, **2020**, 299, 112121	6	6
92	Probing relaxation models by means of Fast Field-Cycling relaxometry, NMR spectroscopy and molecular dynamics simulations: Detailed insight into the translational and rotational dynamics of a protic ionic liquid. *Journal of Molecular Liquids*, **2020**, 319, 114207	6	8
91	Isolating the role of hydrogen bonding in hydroxyl-functionalized ionic liquids by means of vaporization enthalpies, infrared spectroscopy and molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2019**, 21, 20308-20314	3.6	7
90	The Double-Faced Nature of Hydrogen Bonding in Hydroxy-Functionalized Ionic Liquids Shown by Neutron Diffraction and Molecular Dynamics Simulations. *Angewandte Chemie - International Edition*, **2019**, 58, 12887-12892	16.4	30
89	Die zweigesichtige Natur der Wasserstoffbr□kenbindung in hydroxylfunktionalisierten ionischen Fl□ssigkeiten, offenbart durch Neutronendiffraktometrie und Molekulardynamik-Simulation. *Angewandte Chemie*, **2019**, 131, 13019-13024	3.6	3
88	Hydrogen Bonding Between Ions of Like Charge in Ionic Liquids Characterized by NMR Deuteron Quadrupole Coupling Constants□omparison with Salt Bridges and Molecular Systems. *Angewandte Chemie*, **2019**, 131, 18027-18035	3.6	3
87	Hydrogen Bonding Between Ions of Like Charge in Ionic Liquids Characterized by NMR Deuteron Quadrupole Coupling Constants-Comparison with Salt Bridges and Molecular Systems. *Angewandte Chemie - International Edition*, **2019**, 58, 17863-17871	16.4	28
86	Simultaneous determination of deuteron quadrupole coupling constants and rotational correlation times: the model case of hydrogen bonded ionic liquids. *Physical Chemistry Chemical Physics*, **2019**, 21, 25597-25605	3.6	4
85	Revisiting imidazolium based ionic liquids: Effect of the conformation bias of the [NTf] anion studied by molecular dynamics simulations. *Journal of Chemical Physics*, **2018**, 148, 193828	3.9	34

84	Rotational and translational dynamics and their relation to hydrogen bond lifetimes in an ionic liquid by means of NMR relaxation time experiments and molecular dynamics simulation. *Journal of Chemical Physics*, **2018**, 148, 193843	3.9	18
83	Dynamical heterogeneities in ionic liquids as revealed from deuteron NMR. *Chemical Communications*, **2018**, 54, 3098-3101	5.8	15
82	The influence of like-charge attraction on the structure and dynamics of ionic liquids: NMR chemical shifts, quadrupole coupling constants, rotational correlation times and failure of Stokes-Einstein-Debye. *Physical Chemistry Chemical Physics*, **2018**, 20, 5617-5625	3.6	19
81	The Relation between Vaporization Enthalpies and Viscosities: Eyring's Theory Applied to Selected Ionic Liquids. *ChemPhysChem*, **2017**, 18, 1242-1246	3.2	9
80	A simple guiding principle for the temperature dependence of the solubility of light gases in imidazolium-based ionic liquids derived from molecular simulations. *Physical Chemistry Chemical Physics*, **2017**, 19, 1770-1780	3.6	16
79	Charakterisierung von Wasserstoffbrücken zwischen Ionen in protischen ionischen Flüssigkeiten mittels NMR-Deuteron-Quadrupol-Kopplungskonstanten – Unterschiede zu H-Brücken in Amiden, Peptiden und Proteinen. *Angewandte Chemie*, **2017**, 129, 14500-14505	3.6	5
78	Characterization of Doubly Ionic Hydrogen Bonds in Protic Ionic Liquids by NMR Deuteron Quadrupole Coupling Constants: Differences to H-bonds in Amides, Peptides, and Proteins. *Angewandte Chemie - International Edition*, **2017**, 56, 14310-14314	16.4	28
77	Operational Criteria for the Separation of Alkanes by Zeolite Membranes. *Chemie-Ingenieur-Technik*, **2017**, 89, 926-934	0.8	4
76	Deuteron quadrupole coupling constants and reorientational correlation times in protic ionic liquids. *Physical Chemistry Chemical Physics*, **2016**, 18, 17788-94	3.6	18
75	Corporate Development with Agile Business Process Modeling as a Key Success Factor. *Procedia Computer Science*, **2016**, 100, 1168-1175	1.6	7
74	Controlling the subtle energy balance in protic ionic liquids: dispersion forces compete with hydrogen bonds. *Angewandte Chemie - International Edition*, **2015**, 54, 2792-5	16.4	71
73	Non-ideal mixing behaviour of hydrogen bonding in mixtures of protic ionic liquids. *ChemPhysChem*, **2015**, 16, 299-304	3.2	41
72	Steuerung der subtilen Energiebalance in protischen ionischen Flüssigkeiten: Dispersionskräfte im Wettstreit mit Wasserstoffbrücken. *Angewandte Chemie*, **2015**, 127, 2834-2837	3.6	12
71	Hydrogen bonding in a mixture of protic ionic liquids: a molecular dynamics simulation study. *Physical Chemistry Chemical Physics*, **2015**, 17, 8431-40	3.6	63
70	Combination of membrane separation and gas condensation for advanced natural gas conditioning. *Journal of Membrane Science*, **2014**, 453, 100-107	9.6	11
69	Advancing into water's "no man's land": two liquid states?. *Angewandte Chemie - International Edition*, **2014**, 53, 11699-701	16.4	8
68	Angriff auf das „Niemandsland" des Wassers: Zwei Flüssigkeiten?. *Angewandte Chemie*, **2014**, 126, 11888-11890	3.6	2
67	Desorption-controlled separation of natural gas alkanes by zeolite membranes. *RSC Advances*, **2014**, 4, 59831-59834	3.7	8

66	The Influence of Water on the Solubility of Carbon Dioxide in Imidazolium Based Ionic Liquids. *Zeitschrift Fur Physikalische Chemie*, **2013**, 227, 167-176	3.1	16
65	Abreicherung von Flüssiggas aus Erdgas mittels Zeolithmembranen. *Chemie-Ingenieur-Technik*, **2013**, 85, 713-722	0.8	3
64	MFI Membranes for the Separation of Liquefied Petroleum Gas from Methane. *Procedia Engineering*, **2012**, 44, 1138-1140		
63	Activity Coefficients of Complex Molecules by Molecular Simulation and Gibbs-Duhem Integration. *Soft Materials*, **2012**, 10, 26-41	1.7	18
62	The effect of neutral ion aggregate formation on the electrical conductivity of an ionic liquid and its mixtures with chloroform. *ChemPhysChem*, **2012**, 13, 1748-52	3.2	29
61	Cavity model challenged: the hydrated electron is localized in regions of enhanced water density. *ChemPhysChem*, **2011**, 12, 75-7	3.2	5
60	Understanding the dissolution of polyols by ionic liquids using the example of a well-defined model compound. *ChemPhysChem*, **2011**, 12, 2400-4	3.2	20
59	Ionenabhängige Struktur und Dynamik von Wassermolekülen jenseits der ersten Hydrathülle. *Angewandte Chemie*, **2011**, 123, 368-370	3.6	11
58	Der Einfluss von Wasserstoffbrückendefekten auf die Eigenschaften ionischer Flüssigkeiten. *Angewandte Chemie*, **2011**, 123, 6791-6795	3.6	27
57	Specific ion effects on water structure and dynamics beyond the first hydration shell. *Angewandte Chemie - International Edition*, **2011**, 50, 352-3	16.4	71
56	The influence of hydrogen-bond defects on the properties of ionic liquids. *Angewandte Chemie - International Edition*, **2011**, 50, 6661-5	16.4	104
55	Influence of water-protein hydrogen bonding on the stability of Trp-cage miniprotein. A comparison between the TIP3P and TIP4P-Ew water models. *Physical Chemistry Chemical Physics*, **2011**, 13, 19840-7	3.6	63
54	More accurate X-ray scattering data of deeply supercooled bulk liquid water. *Molecular Physics*, **2011**, 109, 279-288	1.7	38
53	Equilibrium study of protein denaturation by urea. *Journal of the American Chemical Society*, **2010**, 132, 2338-44	16.4	218
52	Microsecond simulations of the folding/unfolding thermodynamics of the Trp-cage miniprotein. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 1889-99	4.2	158
51	Tetrahydrofuran clathrate hydrate formation. *Physical Review Letters*, **2009**, 103, 218301	7.4	43
50	Applying the inductive effect for synthesizing low-melting and low-viscosity imidazolium-based ionic liquids. *ChemPhysChem*, **2009**, 10, 516-9	3.2	21
49	Temperature dependence of the solubility of carbon dioxide in imidazolium-based ionic liquids. *Journal of Physical Chemistry B*, **2009**, 113, 12727-35	3.4	92

48	How Does Solute-Polarization Affect the Hydrophobic Hydration of Methane?. *Zeitschrift Fur Physikalische Chemie*, **2009**, 223, 1091-1104	3.1	8
47	Water, Properties of **2008**, 1		1
46	Simulation of the pressure and temperature folding/unfolding equilibrium of a small RNA hairpin. *Journal of the American Chemical Society*, **2008**, 130, 815-7	16.4	124
45	Modeling of aqueous poly(oxyethylene) solutions: 1. Atomistic simulations. *Journal of Physical Chemistry B*, **2008**, 112, 2388-98	3.4	75
44	Modeling of aqueous poly(oxyethylene) solutions. 2. Mesoscale simulations. *Journal of Physical Chemistry B*, **2008**, 112, 13561-71	3.4	51
43	Computing the stability diagram of the Trp-cage miniprotein. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 17754-9	11.5	133
42	Solvophobic solvation and interaction of small apolar particles in imidazolium-based ionic liquids. *Physical Review Letters*, **2008**, 100, 115901	7.4	18
41	Computing Activity Coefficients of Binary Lennard-Jones Mixtures by Gibbs-Duhem Integration. *Zeitschrift Fur Physikalische Chemie*, **2008**, 222, 687-694	3.1	5
40	Ionic liquids: dissecting the enthalpies of vaporization. *ChemPhysChem*, **2008**, 9, 549-55	3.2	117
39	On the validity of Stokes-Einstein and Stokes-Einstein-Debye relations in ionic liquids and ionic-liquid mixtures. *ChemPhysChem*, **2008**, 9, 1851-8	3.2	127
38	Thermodynamic and structural characterization of the transformation from a metastable low-density to a very high-density form of supercooled TIP4P-Ew model water. *ChemPhysChem*, **2008**, 9, 2737-41	3.2	51
37	The solvent-dependent shift of the amide I band of a fully solvated peptide as a local probe for the solvent composition in the peptide/solvent interface. *ChemPhysChem*, **2008**, 9, 2742-50	3.2	11
36	Temperature and concentration effects on the solvophobic solvation of methane in aqueous salt solutions. *ChemPhysChem*, **2008**, 9, 2722-30	3.2	12
35	Pressure and salt effects in simulated water: two sides of the same coin?. *Angewandte Chemie - International Edition*, **2007**, 46, 8907-11	16.4	76
34	Druck- und Salzeffekte in simuliertem Wasser: zwei Seiten einer Medaille?. *Angewandte Chemie*, **2007**, 119, 9065-9069	3.6	10
33	Molecular dynamic simulations of ionic liquids: a reliable description of structure, thermodynamics and dynamics. *ChemPhysChem*, **2007**, 8, 2464-70	3.2	316
32	Replica exchange simulation of reversible folding/unfolding of the Trp-cage miniprotein in explicit solvent: on the structure and possible role of internal water. *Journal of Structural Biology*, **2007**, 157, 524-33	3.4	105
31	Chapter 5 Simulations of Temperature and Pressure Unfolding of Peptides and Proteins with Replica Exchange Molecular Dynamics. *Annual Reports in Computational Chemistry*, **2006**, 83-95	1.8	35

30	Adding salt to an aqueous solution of t-butanol: is hydrophobic association enhanced or reduced?. *Journal of Chemical Physics*, **2006**, 124, 154508	3.9	14
29	Solubility of simple, nonpolar compounds in TIP4P-Ew. *Journal of Chemical Physics*, **2006**, 124, 16102	3.9	20
28	Spatial correlations of interatomic voids in molecular liquids studied using Delaunay simplices. *Journal of Structural Chemistry*, **2006**, 47, S119-S125	0.9	2
27	Low-temperature and high-pressure induced swelling of a hydrophobic polymer-chain in aqueous solution. *Physical Chemistry Chemical Physics*, **2005**, 7, 2780-6	3.6	38
26	Wasser: Anomalien und RÆtsel. *Chemie in Unserer Zeit*, **2005**, 39, 164-175	0.2	16
25	How the liquid-liquid transition affects hydrophobic hydration in deeply supercooled water. *Physical Review Letters*, **2005**, 94, 217802	7.4	160
24	Simulations of the pressure and temperature unfolding of an alpha-helical peptide. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 6765-70	11.5	103
23	Heat capacity effects associated with the hydrophobic hydration and interaction of simple solutes: a detailed structural and energetical analysis based on molecular dynamics simulations. *Journal of Chemical Physics*, **2004**, 120, 10605-17	3.9	69
22	Temperature dependence of the hydrophobic hydration and interaction of simple solutes: an examination of five popular water models. *Journal of Chemical Physics*, **2004**, 120, 6674-90	3.9	241
21	Modeling the occupancy dependence of diffusivities in zeolites. *Microporous and Mesoporous Materials*, **2004**, 76, 233-246	5.3	92
20	Reversible temperature and pressure denaturation of a protein fragment: a replica exchange molecular dynamics simulation study. *Physical Review Letters*, **2004**, 93, 238105	7.4	132
19	Phase coexistence and dynamic properties of water in nanopores. *European Physical Journal E*, **2003**, 12, 69-76	1.5	54
18	Mechanisms of the molecular mobility of water. *Journal of Molecular Liquids*, **2003**, 106, 131-146	6	45
17	Verification of the Maxwell–Stefan theory for tracer diffusion in zeolites. *Chemical Engineering Journal*, **2002**, 85, 7-15	14.7	31
16	Self-diffusivities in multicomponent mixtures in zeolites. *Physical Chemistry Chemical Physics*, **2002**, 4, 1891-1898	3.6	68
15	Simulation of confined water in equilibrium with a bulk reservoir. *Fluid Phase Equilibria*, **2001**, 183-184, 331-339	2.5	19
14	Monte Carlo simulations of sorption and diffusion of isobutane in silicalite. *Chemical Physics Letters*, **2001**, 342, 148-154	2.5	30
13	Inter-relation between self- and jump-diffusivities in zeolites. *Chemical Physics Letters*, **2001**, 333, 278-284	2.5	44

12	Molecular simulations of adsorption and siting of light alkanes in silicalite-1. *Physical Chemistry Chemical Physics*, **2001**, 3, 453-462	3.6	63
11	Kinetic Monte Carlo simulations of transport diffusivities of binary mixtures in zeolites. *Physical Chemistry Chemical Physics*, **2001**, 3, 3185-3191	3.6	36
10	Diffusion of Binary Mixtures in Zeolites: Kinetic Monte Carlo versus Molecular Dynamics Simulations. *Langmuir*, **2001**, 17, 247-254	4	56
9	Separation of hydrocarbon mixtures using zeolite membranes: a modelling approach combining molecular simulations with the Maxwell–Stefan theory. *Separation and Purification Technology*, **2000**, 21, 111-136	8.3	84
8	Gibbs ensemble simulation of water in spherical cavities. *Journal of Chemical Physics*, **2000**, 113, 5026	3.9	60
7	Electrostatic properties of cyano-containing mesogens. *Liquid Crystals*, **2000**, 27, 1137-1146	2.3	10
6	Monte Carlo simulations of self- and transport-diffusivities of 2-methylhexane in silicalite. *Physical Chemistry Chemical Physics*, **2000**, 2, 2389-2394	3.6	55
5	Permeation of Hexane Isomers across ZSM-5 Zeolite Membranes. *Industrial & Engineering Chemistry Research*, **2000**, 39, 2618-2622	3.9	38
4	MD-simulation study of the hydrophobic hydration of nonionic surfactants. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **1999**, 156, 489-500	5.1	8
3	Simulation Study on the Diffusive Motion in Deeply Supercooled Water. *Journal of Physical Chemistry B*, **1999**, 103, 4139-4146	3.4	70
2	Atomistic modelling of ferroelectric liquid crystals. *Ferroelectrics*, **1998**, 212, 45-53	0.6	3
1	Simulation Studies of the Adsorption of Xenon on the (110) Face of Rutile. *Langmuir*, **1995**, 11, 3097-3102	4	15