

Dietmar Paschek

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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	Molecular dynamic simulations of ionic liquids: a reliable description of structure, thermodynamics and dynamics. <i>ChemPhysChem</i> , 2007 , 8, 2464-70	3.2	316
100	Temperature dependence of the hydrophobic hydration and interaction of simple solutes: an examination of five popular water models. <i>Journal of Chemical Physics</i> , 2004 , 120, 6674-90	3.9	241
99	Equilibrium study of protein denaturation by urea. <i>Journal of the American Chemical Society</i> , 2010 , 132, 2338-44	16.4	218
98	How the liquid-liquid transition affects hydrophobic hydration in deeply supercooled water. <i>Physical Review Letters</i> , 2005 , 94, 217802	7.4	160
97	Microsecond simulations of the folding/unfolding thermodynamics of the Trp-cage miniprotein. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010 , 78, 1889-99	4.2	158
96	Computing the stability diagram of the Trp-cage miniprotein. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008 , 105, 17754-9	11.5	133
95	Reversible temperature and pressure denaturation of a protein fragment: a replica exchange molecular dynamics simulation study. <i>Physical Review Letters</i> , 2004 , 93, 238105	7.4	132
94	On the validity of Stokes-Einstein and Stokes-Einstein-Debye relations in ionic liquids and ionic-liquid mixtures. <i>ChemPhysChem</i> , 2008 , 9, 1851-8	3.2	127
93	Simulation of the pressure and temperature folding/unfolding equilibrium of a small RNA hairpin. <i>Journal of the American Chemical Society</i> , 2008 , 130, 815-7	16.4	124
92	Ionic liquids: dissecting the enthalpies of vaporization. <i>ChemPhysChem</i> , 2008 , 9, 549-55	3.2	117
91	Replica exchange simulation of reversible folding/unfolding of the Trp-cage miniprotein in explicit solvent: on the structure and possible role of internal water. <i>Journal of Structural Biology</i> , 2007 , 157, 524-33	3.4	105
90	The influence of hydrogen-bond defects on the properties of ionic liquids. <i>Angewandte Chemie - International Edition</i> , 2011 , 50, 6661-5	16.4	104
89	Simulations of the pressure and temperature unfolding of an alpha-helical peptide. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005 , 102, 6765-70	11.5	103
88	Temperature dependence of the solubility of carbon dioxide in imidazolium-based ionic liquids. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 12727-35	3.4	92
87	Modeling the occupancy dependence of diffusivities in zeolites. <i>Microporous and Mesoporous Materials</i> , 2004 , 76, 233-246	5.3	92
86	Separation of hydrocarbon mixtures using zeolite membranes: a modelling approach combining molecular simulations with the Maxwell-Stefan theory. <i>Separation and Purification Technology</i> , 2000 , 21, 111-136	8.3	84
85	Pressure and salt effects in simulated water: two sides of the same coin?. <i>Angewandte Chemie - International Edition</i> , 2007 , 46, 8907-11	16.4	76

84	Modeling of aqueous poly(oxyethylene) solutions: 1. Atomistic simulations. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 2388-98	3.4	75
83	Controlling the subtle energy balance in protic ionic liquids: dispersion forces compete with hydrogen bonds. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 2792-5	16.4	71
82	Specific ion effects on water structure and dynamics beyond the first hydration shell. <i>Angewandte Chemie - International Edition</i> , 2011 , 50, 352-3	16.4	71
81	Simulation Study on the Diffusive Motion in Deeply Supercooled Water. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 4139-4146	3.4	70
80	Heat capacity effects associated with the hydrophobic hydration and interaction of simple solutes: a detailed structural and energetical analysis based on molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2004 , 120, 10605-17	3.9	69
79	Self-diffusivities in multicomponent mixtures in zeolites. <i>Physical Chemistry Chemical Physics</i> , 2002 , 4, 1891-1898	3.6	68
78	Hydrogen bonding in a mixture of protic ionic liquids: a molecular dynamics simulation study. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 8431-40	3.6	63
77	Influence of water-protein hydrogen bonding on the stability of Trp-cage miniprotein. A comparison between the TIP3P and TIP4P-Ew water models. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 19840-7	3.6	63
76	Molecular simulations of adsorption and siting of light alkanes in silicalite-1. <i>Physical Chemistry Chemical Physics</i> , 2001 , 3, 453-462	3.6	63
75	Gibbs ensemble simulation of water in spherical cavities. <i>Journal of Chemical Physics</i> , 2000 , 113, 5026	3.9	60
74	Diffusion of Binary Mixtures in Zeolites: Kinetic Monte Carlo versus Molecular Dynamics Simulations. <i>Langmuir</i> , 2001 , 17, 247-254	4	56
73	Monte Carlo simulations of self- and transport-diffusivities of 2-methylhexane in silicalite. <i>Physical Chemistry Chemical Physics</i> , 2000 , 2, 2389-2394	3.6	55
72	Phase coexistence and dynamic properties of water in nanopores. <i>European Physical Journal E</i> , 2003 , 12, 69-76	1.5	54
71	Modeling of aqueous poly(oxyethylene) solutions. 2. Mesoscale simulations. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 13561-71	3.4	51
70	Thermodynamic and structural characterization of the transformation from a metastable low-density to a very high-density form of supercooled TIP4P-Ew model water. <i>ChemPhysChem</i> , 2008 , 9, 2737-41	3.2	51
69	Mechanisms of the molecular mobility of water. <i>Journal of Molecular Liquids</i> , 2003 , 106, 131-146	6	45
68	Inter-relation between self- and jump-diffusivities in zeolites. <i>Chemical Physics Letters</i> , 2001 , 333, 278-284	5	44
67	Tetrahydrofuran clathrate hydrate formation. <i>Physical Review Letters</i> , 2009 , 103, 218301	7.4	43

66	Non-ideal mixing behaviour of hydrogen bonding in mixtures of protic ionic liquids. <i>ChemPhysChem</i> , 2015 , 16, 299-304	3.2	41
65	More accurate X-ray scattering data of deeply supercooled bulk liquid water. <i>Molecular Physics</i> , 2011 , 109, 279-288	1.7	38
64	Low-temperature and high-pressure induced swelling of a hydrophobic polymer-chain in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2005 , 7, 2780-6	3.6	38
63	Permeation of Hexane Isomers across ZSM-5 Zeolite Membranes. <i>Industrial & Engineering Chemistry Research</i> , 2000 , 39, 2618-2622	3.9	38
62	Kinetic Monte Carlo simulations of transport diffusivities of binary mixtures in zeolites. <i>Physical Chemistry Chemical Physics</i> , 2001 , 3, 3185-3191	3.6	36
61	Chapter 5 Simulations of Temperature and Pressure Unfolding of Peptides and Proteins with Replica Exchange Molecular Dynamics. <i>Annual Reports in Computational Chemistry</i> , 2006 , 83-95	1.8	35
60	Revisiting imidazolium based ionic liquids: Effect of the conformation bias of the [NTF] anion studied by molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2018 , 148, 193828	3.9	34
59	Verification of the Maxwell-Stefan theory for tracer diffusion in zeolites. <i>Chemical Engineering Journal</i> , 2002 , 85, 7-15	14.7	31
58	The Double-Faced Nature of Hydrogen Bonding in Hydroxy-Functionalized Ionic Liquids Shown by Neutron Diffraction and Molecular Dynamics Simulations. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 12887-12892	16.4	30
57	Monte Carlo simulations of sorption and diffusion of isobutane in silicalite. <i>Chemical Physics Letters</i> , 2001 , 342, 148-154	2.5	30
56	The effect of neutral ion aggregate formation on the electrical conductivity of an ionic liquid and its mixtures with chloroform. <i>ChemPhysChem</i> , 2012 , 13, 1748-52	3.2	29
55	Hydrogen Bonding Between Ions of Like Charge in Ionic Liquids Characterized by NMR Deuteron Quadrupole Coupling Constants-Comparison with Salt Bridges and Molecular Systems. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 17863-17871	16.4	28
54	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. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 14310-14314	16.4	28
53	Der Einfluss von Wasserstoffbrückendefekten auf die Eigenschaften ionischer Flüssigkeiten. <i>Angewandte Chemie</i> , 2011 , 123, 6791-6795	3.6	27
52	Applying the inductive effect for synthesizing low-melting and low-viscosity imidazolium-based ionic liquids. <i>ChemPhysChem</i> , 2009 , 10, 516-9	3.2	21
51	Understanding the dissolution of polyols by ionic liquids using the example of a well-defined model compound. <i>ChemPhysChem</i> , 2011 , 12, 2400-4	3.2	20
50	Solubility of simple, nonpolar compounds in TIP4P-Ew. <i>Journal of Chemical Physics</i> , 2006 , 124, 16102	3.9	20
49	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. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 5617-5625	3.6	19

48	Simulation of confined water in equilibrium with a bulk reservoir. <i>Fluid Phase Equilibria</i> , 2001 , 183-184, 331-339	2.5	19
47	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. <i>Journal of Chemical Physics</i> , 2018 , 148, 193843	3.9	18
46	Activity Coefficients of Complex Molecules by Molecular Simulation and Gibbs-Duhem Integration. <i>Soft Materials</i> , 2012 , 10, 26-41	1.7	18
45	Solvophobic solvation and interaction of small apolar particles in imidazolium-based ionic liquids. <i>Physical Review Letters</i> , 2008 , 100, 115901	7.4	18
44	Deuteron quadrupole coupling constants and reorientational correlation times in protic ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 17788-94	3.6	18
43	A simple guiding principle for the temperature dependence of the solubility of light gases in imidazolium-based ionic liquids derived from molecular simulations. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 1770-1780	3.6	16
42	The Influence of Water on the Solubility of Carbon Dioxide in Imidazolium Based Ionic Liquids. <i>Zeitschrift Fur Physikalische Chemie</i> , 2013 , 227, 167-176	3.1	16
41	Wasser: Anomalien und Rätsel. <i>Chemie in Unserer Zeit</i> , 2005 , 39, 164-175	0.2	16
40	Dynamical heterogeneities in ionic liquids as revealed from deuteron NMR. <i>Chemical Communications</i> , 2018 , 54, 3098-3101	5.8	15
39	Simulation Studies of the Adsorption of Xenon on the (110) Face of Rutile. <i>Langmuir</i> , 1995 , 11, 3097-3107	1.7	15
38	Adding salt to an aqueous solution of t-butanol: is hydrophobic association enhanced or reduced?. <i>Journal of Chemical Physics</i> , 2006 , 124, 154508	3.9	14
37	Steuerung der subtilen Energiebalance in protischen ionischen Flüssigkeiten: Dispersionskräfte im Wettstreit mit Wasserstoffbrücken. <i>Angewandte Chemie</i> , 2015 , 127, 2834-2837	3.6	12
36	Temperature and concentration effects on the solvophobic solvation of methane in aqueous salt solutions. <i>ChemPhysChem</i> , 2008 , 9, 2722-30	3.2	12
35	Combination of membrane separation and gas condensation for advanced natural gas conditioning. <i>Journal of Membrane Science</i> , 2014 , 453, 100-107	9.6	11
34	Ionenabhängige Struktur und Dynamik von Wassermolekülen jenseits der ersten Hydrathülle. <i>Angewandte Chemie</i> , 2011 , 123, 368-370	3.6	11
33	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. <i>ChemPhysChem</i> , 2008 , 9, 2742-50	3.2	11
32	Druck- und Salzeffekte in simuliertem Wasser: zwei Seiten einer Medaille?. <i>Angewandte Chemie</i> , 2007 , 119, 9065-9069	3.6	10
31	Electrostatic properties of cyano-containing mesogens. <i>Liquid Crystals</i> , 2000 , 27, 1137-1146	2.3	10

30	The Relation between Vaporization Enthalpies and Viscosities: Eyring's Theory Applied to Selected Ionic Liquids. <i>ChemPhysChem</i> , 2017 , 18, 1242-1246	3.2	9
29	Counting cations involved in cationic clusters of hydroxy-functionalized ionic liquids by means of infrared and solid-state NMR spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 6861-6867	3.6	9
28	Advancing into water's "no man's land": two liquid states?. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 11699-701	16.4	8
27	Desorption-controlled separation of natural gas alkanes by zeolite membranes. <i>RSC Advances</i> , 2014 , 4, 59831-59834	3.7	8
26	How Does Solute-Polarization Affect the Hydrophobic Hydration of Methane?. <i>Zeitschrift Fur Physikalische Chemie</i> , 2009 , 223, 1091-1104	3.1	8
25	MD-simulation study of the hydrophobic hydration of nonionic surfactants. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 1999 , 156, 489-500	5.1	8
24	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. <i>Journal of Molecular Liquids</i> , 2020 , 319, 114207	6	8
23	Isolating the role of hydrogen bonding in hydroxyl-functionalized ionic liquids by means of vaporization enthalpies, infrared spectroscopy and molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 20308-20314	3.6	7
22	Corporate Development with Agile Business Process Modeling as a Key Success Factor. <i>Procedia Computer Science</i> , 2016 , 100, 1168-1175	1.6	7
21	Comparing the void space and long-range structure of an ionic liquid with a neutral mixture of similar sized molecules. <i>Journal of Molecular Liquids</i> , 2020 , 299, 112121	6	6
20	Charakterisierung von Wasserstoffbrücken zwischen Ionen in protischen ionischen Flüssigkeiten mittels NMR-Deuteron-Quadrupol-Kopplungskonstanten Δ Unterschiede zu H-Brücken in Amiden, Peptiden und Proteinen. <i>Angewandte Chemie</i> , 2017 , 129, 14500-14505	3.6	5
19	Cavity model challenged: the hydrated electron is localized in regions of enhanced water density. <i>ChemPhysChem</i> , 2011 , 12, 75-7	3.2	5
18	Computing Activity Coefficients of Binary Lennard-Jones Mixtures by Gibbs-Duhem Integration. <i>Zeitschrift Fur Physikalische Chemie</i> , 2008 , 222, 687-694	3.1	5
17	Kinetics of Hydrogen Bonding between Ions with Opposite and Like Charges in Hydroxyl-Functionalized Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 281-286	3.4	5
16	Operational Criteria for the Separation of Alkanes by Zeolite Membranes. <i>Chemie-Ingenieur-Technik</i> , 2017 , 89, 926-934	0.8	4
15	Structural similarity of an ionic liquid and the mixture of the neutral molecules. <i>Journal of Molecular Liquids</i> , 2021 , 329, 115589	6	4
14	Simultaneous determination of deuteron quadrupole coupling constants and rotational correlation times: the model case of hydrogen bonded ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 25597-25605	3.6	4
13	Quasi-Universal Solubility Behavior of Light Gases in Imidazolium-Based Ionic Liquids with Varying Anions: A Molecular Dynamics Simulation Study. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 1647-1659	3.4	4

12	Die zweigesichtige Natur der Wasserstoffbrückenbindung in hydroxylfunktionalisierten ionischen Flüssigkeiten, offenbart durch Neutronendiffraktometrie und Molekulardynamik-Simulation. <i>Angewandte Chemie</i> , 2019 , 131, 13019-13024	3.6	3
11	Hydrogen Bonding Between Ions of Like Charge in Ionic Liquids Characterized by NMR Deuteron Quadrupole Coupling Constants—Comparison with Salt Bridges and Molecular Systems. <i>Angewandte Chemie</i> , 2019 , 131, 18027-18035	3.6	3
10	Abreicherung von Flüssiggas aus Erdgas mittels Zeolithmembranen. <i>Chemie-Ingenieur-Technik</i> , 2013 , 85, 713-722	0.8	3
9	Atomistic modelling of ferroelectric liquid crystals. <i>Ferroelectrics</i> , 1998 , 212, 45-53	0.6	3
8	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. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 4476-4488	3.4	3
7	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. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 5132-5144	3.4	3
6	Angriff auf das Niemandsland des Wassers: Zwei Flüssigkeiten?. <i>Angewandte Chemie</i> , 2014 , 126, 11888-11890	3.0	2
5	Spatial correlations of interatomic voids in molecular liquids studied using Delaunay simplices. <i>Journal of Structural Chemistry</i> , 2006 , 47, S119-S125	0.9	2
4	Water, Properties of 2008 , 1		1
3	Why Do Liquids Mix? The Mixing of Protic Ionic Liquids Sharing the Same Cation Is Apparently Driven by Enthalpy, Not Entropy.. <i>Journal of Physical Chemistry Letters</i> , 2022 , 3556-3561	6.4	0
2	MFI Membranes for the Separation of Liquefied Petroleum Gas from Methane. <i>Procedia Engineering</i> , 2012 , 44, 1138-1140		
1	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. <i>Journal of Chemical Physics</i> , 2021 , 154, 214501	3.9	