Dietmar Paschek

List of Publications by Year
in descending order

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99 papers	4,974 citations	76196 40 h-index	95083 68 g-index
116 all docs	116 docs citations	116 times ranked	4283 citing authors

#	Article	IF	Citations
1	Molecular Dynamic Simulations of Ionic Liquids: A Reliable Description of Structure, Thermodynamics and Dynamics. ChemPhysChem, 2007, 8, 2464-2470.	1.0	355
2	Temperature dependence of the hydrophobic hydration and interaction of simple solutes: An examination of five popular water models. Journal of Chemical Physics, 2004, 120, 6674-6690.	1.2	259
3	Equilibrium Study of Protein Denaturation by Urea. Journal of the American Chemical Society, 2010, 132, 2338-2344.	6.6	247
4	How the Liquid-Liquid Transition Affects Hydrophobic Hydration in Deeply Supercooled Water. Physical Review Letters, 2005, 94, 217802.	2.9	175
5	Microsecond simulations of the folding/unfolding thermodynamics of the Trpâ€cage miniprotein. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1889-1899.	1.5	166
6	Computing the stability diagram of the Trp-cage miniprotein. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 17754-17759.	3.3	146
7	On the Validity of Stokesâ€“Einstein and Stokesâ€“Einsteinâ€“Debye Relations in Ionic Liquids and Ionicâ€Liquid Mixtures. ChemPhysChem, 2008, 9, 1851-1858.	1.0	142
8	Simulation of the Pressure and Temperature Folding/Unfolding Equilibrium of a Small RNA Hairpin. Journal of the American Chemical Society, 2008, 130, 815-817.	6.6	141
9	Reversible Temperature and Pressure Denaturation of a Protein Fragment: A Replica Exchange Molecular Dynamics Simulation Study. Physical Review Letters, 2004, 93, 238105.	2.9	137
10	Ionic Liquids: Dissecting the Enthalpies of Vaporization. ChemPhysChem, 2008, 9, 549-555.	1.0	123
11	The Influence of Hydrogenâ€Bond Defects on the Properties of Ionic Liquids. Angewandte Chemie - International Edition, 2011, 50, 6661-6665.	7.2	114
12	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, 524-533.	1.3	110
13	Simulations of the pressure and temperature unfolding of an Â-helical peptide. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6765-6770.	3.3	108
14	Temperature Dependence of the Solubility of Carbon Dioxide in Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2009, 113, 12727-12735.	1.2	104
15	Modeling the occupancy dependence of diffusivities in zeolites. Microporous and Mesoporous Materials, 2004, 76, 233-246.	2.2	100
16	Separation of hydrocarbon mixtures using zeolite membranes: a modelling approach combining molecular simulations with the Maxwellâ€“Stefan theory. Separation and Purification Technology, 2000, 21, 111-136.	3.9	95
17	Modeling of Aqueous Poly(oxyethylene) Solutions:â€‰ 1. Atomistic Simulations. Journal of Physical Chemistry B, 2008, 112, 2388-2398.	1.2	83
18	Pressure and Salt Effects in Simulated Water: Two Sides of the Same Coin?. Angewandte Chemie - International Edition, 2007, 46, 8907-8911.	7.2	79

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19	Specific Ion Effects on Water Structure and Dynamics beyond the First Hydration Shell. Angewandte Chemie - International Edition, 2011, 50, 352-353.	7.2	78
20	Controlling the Subtle Energy Balance in Protic Ionic Liquids: Dispersion Forces Compete with Hydrogen Bonds. Angewandte Chemie - International Edition, 2015, 54, 2792-2795.	7.2	78
21	Simulation Study on the Diffusive Motion in Deeply Supercooled Water. Journal of Physical Chemistry B, 1999, 103, 4139-4146.	1.2	76
22	Hydrogen bonding in a mixture of protic ionic liquids: a molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2015, 17, 8431-8440.	1.3	74
23	Self-diffusivities in multicomponent mixtures in zeolites. Physical Chemistry Chemical Physics, 2002, 4, 1891-1898.	1.3	73
24	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, 10605-10617.	1.2	71
25	Molecular simulations of adsorption and siting of light alkanes in silicalite-1. Physical Chemistry Chemical Physics, 2001, 3, 453-462.	1.3	70
26	Influence of waterâ€“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.	1.3	69
27	Gibbs ensemble simulation of water in spherical cavities. Journal of Chemical Physics, 2000, 113, 5026.	1.2	65
28	Diffusion of Binary Mixtures in Zeolites:Â Kinetic Monte Carlo versus Molecular Dynamics Simulations. Langmuir, 2001, 17, 247-254.	1.6	65
29	Monte Carlo simulations of self- and transport-diffusivities of 2-methylhexane in silicalite. Physical Chemistry Chemical Physics, 2000, 2, 2389-2394.	1.3	62
30	Thermodynamic and Structural Characterization of the Transformation from a Metastable Lowâ€Density to a Very Highâ€Density Form of Supercooled TIP4Pâ€Ew Model Water. ChemPhysChem, 2008, 9, 2737-2741.	1.0	56
31	Phase coexistence and dynamic properties of water in nanopores. European Physical Journal E, 2003, 12, 69-76.	0.7	55
32	Modeling of Aqueous Poly(oxyethylene) Solutions. 2. Mesoscale Simulations. Journal of Physical Chemistry B, 2008, 112, 13561-13571.	1.2	55
33	Inter-relation between self- and jump-diffusivities in zeolites. Chemical Physics Letters, 2001, 333, 278-284.	1.2	51
34	Tetrahydrofuran Clathrate Hydrate Formation. Physical Review Letters, 2009, 103, 218301.	2.9	50
35	Nonâ€Ideal Mixing Behaviour of Hydrogen Bonding in Mixtures of Protic Ionic Liquids. ChemPhysChem, 2015, 16, 299-304.	1.0	50
36	Mechanisms of the molecular mobility of water. Journal of Molecular Liquids, 2003, 106, 131-146.	2.3	47

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37	Permeation of Hexane Isomers across ZSM-5 Zeolite Membranes. Industrial & Engineering Chemistry Research, 2000, 39, 2618-2622.	1.8	42
38	Revisiting imidazolium based ionic liquids: Effect of the conformation bias of the [NTf2] anion studied by molecular dynamics simulations. Journal of Chemical Physics, 2018, 148, 193828.	1.2	42
39	Kinetic Monte Carlo simulations of transport diffusivities of binary mixtures in zeolites. Physical Chemistry Chemical Physics, 2001, 3, 3185-3191.	1.3	41
40	More accurate X-ray scattering data of deeply supercooled bulk liquid water. Molecular Physics, 2011, 109, 279-288.	0.8	41
41	Hydrogen Bonding Between Ions of Like Charge in Ionic Liquids Characterized by NMR Deuteron Quadrupole Coupling Constantsâ€"Comparison with Salt Bridges and Molecular Systems. Angewandte Chemie - International Edition, 2019, 58, 17863-17871.	7.2	41
42	The Doubleâ€Faced Nature of Hydrogen Bonding in Hydroxyâ€Functionalized Ionic Liquids Shown by Neutron Diffraction and Molecular Dynamics Simulations. Angewandte Chemie - International Edition, 2019, 58, 12887-12892.	7.2	40
43	Low-temperature and high-pressure induced swelling of a hydrophobic polymer-chain in aqueous solution. Physical Chemistry Chemical Physics, 2005, 7, 2780.	1.3	39
44	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.	0.9	38
45	Characterization of Doubly Ionic Hydrogen Bonds in Protic Ionic Liquids by NMR Deuteron Quadrupole Coupling Constants: Differences to Hâ€bonds in Amides, Peptides, and Proteins. Angewandte Chemie - International Edition, 2017, 56, 14310-14314.	7.2	35
46	Monte Carlo simulations of sorption and diffusion of isobutane in silicalite. Chemical Physics Letters, 2001, 342, 148-154.	1.2	33
47	Verification of the Maxwellâ€"Stefan theory for tracer diffusion in zeolites. Chemical Engineering Journal, 2002, 85, 7-15.	6.6	33
48	The Effect of Neutral Ion Aggregate Formation on the Electrical Conductivity of an Ionic Liquid and its Mixtures with Chloroform. ChemPhysChem, 2012, 13, 1748-1752.	1.0	29
49	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.	1.3	29
50	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 Stokesâ€"Einsteinâ€"Debye. Physical Chemistry Chemical Physics, 2018, 20, 5617-5625.	1.3	26
51	Solubility of simple, nonpolar compounds in TIP4P-Ew. Journal of Chemical Physics, 2006, 124, 016102.	1.2	25
52	Activity Coefficients of Complex Molecules by Molecular Simulation and Gibbs-Duhem Integration. Soft Materials, 2012, 10, 26-41.	0.8	24
53	Deuteron quadrupole coupling constants and reorientational correlation times in protic ionic liquids. Physical Chemistry Chemical Physics, 2016, 18, 17788-17794.	1.3	24
54	Applying the Inductive Effect for Synthesizing Lowâ€Melting and Lowâ€Viscosity Imidazoliumâ€Based Ionic Liquids. ChemPhysChem, 2009, 10, 516-519.	1.0	22

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55	Understanding the Dissolution of Polyols by Ionic Liquids Using the Example of a Wellâ€Defined Model Compound. ChemPhysChem, 2011, 12, 2400-2404.	1.0	22
56	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.	1.2	22
57	Dynamical heterogeneities in ionic liquids as revealed from deuteron NMR. Chemical Communications, 2018, 54, 3098-3101.	2.2	21
58	Simulation of confined water in equilibrium with a bulk reservoir. Fluid Phase Equilibria, 2001, 183-184, 331-339.	1.4	20
59	Wasser: Anomalien und RÃtsel. Chemie in Unserer Zeit, 2005, 39, 164-175.	0.1	19
60	Solvophobic Solvation and Interaction of Small Apolar Particles in Imidazolium-Based Ionic Liquids. Physical Review Letters, 2008, 100, 115901.	2.9	19
61	Adding salt to an aqueous solution of t-butanol: Is hydrophobic association enhanced or reduced?. Journal of Chemical Physics, 2006, 124, 154508.	1.2	17
62	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.	1.3	17
63	The Influence of Water on the Solubility of Carbon Dioxide in Imidazolium Based Ionic Liquids. Zeitschrift Fur Physikalische Chemie, 2013, 227, 167-176.	1.4	16
64	Simulation Studies of the Adsorption of Xenon on the (110) Face of Rutile. Langmuir, 1995, 11, 3097-3102.	1.6	15
65	The Solventâ€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, 2742-2750.	1.0	15
66	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.	1.2	15
67	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.	1.2	15
68	Temperature and Concentration Effects on the Solvophobic Solvation of Methane in Aqueous Salt Solutions. ChemPhysChem, 2008, 9, 2722-2730.	1.0	14
69	Combination of membrane separation and gas condensation for advanced natural gas conditioning. Journal of Membrane Science, 2014, 453, 100-107.	4.1	14
70	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.	1.3	14
71	Steuerung der subtilen Energiebalance in protischen ionischen FlÃ¼ssigkeiten: DispersionskrÃfte im Wettstreit mit WasserstoffbrÃ¼cken. Angewandte Chemie, 2015, 127, 2834-2837.	1.6	13
72	Operational Criteria for the Separation of Alkanes by Zeolite Membranes. Chemie-Ingenieur-Technik, 2017, 89, 926-934.	0.4	13

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73	The Relation between Vaporization Enthalpies and Viscosities: Eyring's Theory Applied to Selected Ionic Liquids. ChemPhysChem, 2017, 18, 1242-1246.	1.0	12
74	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.	2.3	12
75	Electrostatic properties of cyano-containing mesogens. Liquid Crystals, 2000, 27, 1137-1146.	0.9	11
76	Advancing into Waterâ€™s â€œNo Manâ€™s Landâ€: Two Liquid States?. Angewandte Chemie - International Edition, 2014, 53, 11699-11701.	7.2	11
77	Corporate Development with Agile Business Process Modeling as a Key Success Factor. Procedia Computer Science, 2016, 100, 1168-1175.	1.2	11
78	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.	1.2	11
79	Desorption-controlled separation of natural gas alkanes by zeolite membranes. RSC Advances, 2014, 4, 59831-59834.	1.7	9
80	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.	2.3	9
81	Balance Between Contact and Solvent-Separated Ion Pairs in Mixtures of the Protic Ionic Liquid [Et₃NH][MeSO₃] with Water Controlled by Water Content and Temperature. Journal of Physical Chemistry B, 2021, 125, 4476-4488.	1.2	9
82	MD-simulation study of the hydrophobic hydration of nonionic surfactants. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 1999, 156, 489-500.	2.3	8
83	How Does Solute-Polarization Affect the Hydrophobic Hydration of Methane?. Zeitschrift Fur Physikalische Chemie, 2009, 223, 1091-1104.	1.4	8
84	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.	1.3	8
85	Hydrogen Bonding Between Ions of Like Charge in Ionic Liquids Characterized by NMR Deuteron Quadrupole Coupling Constantsâ€”Comparison with Salt Bridges and Molecular Systems. Angewandte Chemie, 2019, 131, 18027-18035.	1.6	7
86	Structural similarity of an ionic liquid and the mixture of the neutral molecules. Journal of Molecular Liquids, 2021, 329, 115589.	2.3	7
87	Computing Activity Coefficients of Binary Lennard-Jones Mixtures by Gibbs-Duhem Integration. Zeitschrift Fur Physikalische Chemie, 2008, 222, 687-694.	1.4	5
88	Cavity Model Challenged: The Hydrated Electron is Localized in Regions of Enhanced Water Density. ChemPhysChem, 2011, 12, 75-77.	1.0	5
89	Charakterisierung von WasserstoffbrÃ¼cken zwischen Ionen in protischen ionischen FlÃ¼ssigkeiten mittels NMRâ€Deuteronâ€Quadrupolâ€Kopplungskonstanten â€“ Unterschiede zu Hâ€BrÃ¼cken in Amiden, Peptiden und Proteinen. Angewandte Chemie, 2017, 129, 14500-14505.	1.6	5
90	Die zweigesichtige Natur der WasserstoffbrÃ¼ckenbindung in hydroxylfunktionalisierten ionischen FlÃ¼ssigkeiten, offenbart durch Neutronendiffraktometrie und Molekulardynamikâ€Simulation. Angewandte Chemie, 2019, 131, 13019-13024.	1.6	5

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91	Depletion of Liquefied Petroleum Gas from Natural Gas by Zeolite Membranes. Chemie-Ingenieur-Technik, 2013, 85, 713-722.	0.4	4
92	Atomistic modelling of ferroelectric liquid crystals. Ferroelectrics, 1998, 212, 45-53.	0.3	3
93	Spatial correlations of interatomic voids in molecular liquids studied using Delaunay simplices. Journal of Structural Chemistry, 2006, 47, S119-S125.	0.3	2
94	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.	1.2	2
95	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, 13, 3556-3561.	2.1	2
96	Hydrogen bond redistribution effects in mixtures of protic ionic liquids sharing the same cation: non-ideal mixing with large negative mixing enthalpies. Physical Chemistry Chemical Physics, 2022, 24, 14740-14750.	1.3	2
97	Molecular dynamics simulations of ammonia adsorbed on titanium dioxide (rutile) surfaces. AIP Conference Proceedings, 1995, , .	0.3	1
98	MFI Membranes for the Separation of Liquefied Petroleum Gas from Methane. Procedia Engineering, 2012, 44, 1138-1140.	1.2	0
99	Editorial of Special Issue ELMG/JMLG 2015. Journal of Molecular Liquids, 2017, 226, 1.	2.3	0