List of Publications

May 6, 2024

Dr. Dietmar Paschek

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Theoretische Chemie
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Peer reviewed publications:	100	Papers with	$\geq$ 200 citations	:	3
Sum of the times cited (Scopus):	4809	···	$\geq$ 100 citations	:	14
Average citations per item:	48.09	···	$\geq$ 50 citations	:	34
Citing documents (Scopus):	3580	···	$\geq$ 20 citations	:	61
h-index (Scopus):	**39**	···	$\geq$ 10 citations	:	78

DP Single Author:	4	(4.0 %)	DP Co-Author:	43	(43.0 %)
DP First Author:	23	(23.0 %)	DP* Corresponding Author:	38	(38.0 %)
DP Last Author:	30	(30.0 %)			

Peer Reviewed Publications

100. D. Paschek*, J. Busch, E. Mock, R. Ludwig, A. Strate
"Computing the Frequency Dependent NMR Relaxation of ^{1}H Nuclei in Liquid Water"
J. Chem. Phys. **160**, 074102 (2024).
JCP EP: Editor's Pick
DOI: 10.1063/5.0191052

99. J. Busch, D. Paschek*
"Computing Accurate True Self-Diffusion Coefficients and Shear Viscosities Using the OrthoBoXY-Approach"
J. Phys. Chem. B **128**, 1040-1052 (2024).
DOI: 10.1021/acs.jpcb.3c07540

98. J. Busch, D. Paschek*
"An OrthoBoXY-Method for Various Alternative Box Geometries"
Phys. Chem. Chem. Phys. **26**, 2907-2914 (2024).
2023 PCCP HOT Articles
DOI: 10.1039/D3CP04916G
(1 citation)

2023

97. J. Busch, D. Paschek*
"OrthoBoXY: A Simple Way to Compute True Self-Diffusion Coefficients from MD Simulations with Periodic Boundary Conditions without Prior Knowledge of the Viscosity"
J. Phys. Chem. B **127**, 7983-7987 (2023).
DOI: 10.1021/acs.jpcb.3c04492
(5 citations)

96. A.E. Khudozhitkov, D. Paschek, A.G. Stepanov, D.I. Kolokolov, R. Ludwig
"How Like-Charge Attraction Influences the Mobility of Cations in Hydroxyl-Functionalized Ionic Liquids"
J. Phys. Chem. Lett. **14**, 4019-4025 (2023).
DOI: 10.1021/acs.jpclett.3c00463
(3 citations)

95. J. Busch, T. Niemann, J. Neumann, P. Stange, S. Gärtner, T.G.A. Youngs, S. Youngs, D. Paschek, R. Ludwig
"The role of hydrogen bond defects for cluster formation and distribution in ionic liquids by means of neutron diffraction and molecular dynamics simulations"
ChemPhysChem **24**, e202300031 (2023).
DOI: 10.1002/cphc.202300031
(2 citations)

94. J. Busch, D. Kotwica, L. Al Sheak, T. Headen, T.G.A. Youngs, D. Paschek, R. Ludwig
"Quantification and Distribution of Three Types of Hydrogen Bonds in Mixtures of an Ionic Liquid with the Hydrogen-Bond-Accepting Molecular Solvent DMSO Explored by Neutron Diffraction and Molecular Dynamics Simulations"
J. Phys. Chem. Lett. **14**, 2684-2689 (2023).
DOI: 10.1021/acs.jpclett.3c00018

2022

93. A.E. Khudozhitkov, P. Stange, D. Paschek, A.G. Stepanov, D.I. Kolokolov, R. Ludwig
"The influence of deuterium isotope effects on structural rearrangements, ensemble equilibria, and hydrogen bonding in protic ionic liquids"
ChemPhysChem **23**, e202200557 (2022).

DOI: 10.1002/cphc.202200557
(2 citations)

92. B. Golub, D. Ondo, V. Overbeck, R. Ludwig, D. Paschek*
"Hydrogen Bond Redistribution Effects in Mixtures of Protic Ionic Liquids Sharing the Same Cation: Non-ideal Mixing with Large Negative Mixing Enthalpies"
Phys. Chem. Chem. Phys. **24**, 14740-14750 (2022).
2022 PCCP HOT Articles
DOI: 10.1039/D2CP01209J
(2 citations)

91. B. Golub, D. Ondo, R. Ludwig, D. Paschek*
"Why Do Liquids Mix? The Mixing of Protic Ionic Liquids Sharing the Same Cation is Apparently Driven By Enthalpy, Not Entropy"
J. Phys. Chem. Lett. **13**, 3556-3561 (2022).
DOI: 10.1021/acs.jpclett.2c00634
(2 citations)

2021

90. J. Busch, J. Neumann, D. Paschek*
"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"
J. Chem. Phys. **154**, 214501 (2021).
DOI: 10.1063/5.0053445
(2 citations)

89. J. Neumann, R. Ludwig, D. Paschek*
"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"
J. Phys. Chem. B **125**, 5132-5144 (2021).
DOI: 10.1021/acs.jpcb.1c02756
(11 citations)

88. B. Golub, K. Fumino, P. Stange, V. Fossog, R. Hempelmann, D. Ondo, D. Paschek*, R. Ludwig
"Balance Between Contact and Solvent Separated Ion Pairs in Mixtures of the Protic Ionic Liquid $[Et_3NH][MeSO_3]$ with Water Controlled by Water Content and Temperature "
J. Phys. Chem. B **125**, 4476-4488 (2021).
DOI: 10.1021/acs.jpcb.1c01850
(9 citations)

87. E.A. Shelepova, R. Ludwig, D. Paschek*, N.N. Medvedev
"Structural similarity of an ionic liquid and the mixture of the neutral molecules"
J. Mol. Liq. **329**, 115589 (2021).
Special Issue: EMLG/JMLG Meeting 2019
DOI: 10.1016/j.molliq.2021.115589
(7 citations)

86. M. Namayandeh Jorabchi, R. Ludwig, D. Paschek*
"Quasi-Universal Solubility Behavior of Light Gases in Imidazolium-based Ionic Liquids with Varying Anions: A Molecular Dynamics Simulation Study "
J. Phys. Chem. B **125**, 1647-1659 (2021).
Lawrence R. Pratt Festschrift
DOI: 10.1021/acs.jpcb.0c10721
(16 citations)

85. J. Neumann, D. Paschek, A. Strate, R. Ludwig
"Kinetics of hydrogen bonding between ions with opposite and like charges in hydroxyl-functionalized ionic liquids"
J. Phys. Chem. B **125**, 281-286 (2021).
DOI: 10.1021/acs.jpcb.0c09278
(16 citations)

2020

84. V. Overbeck, B. Golub, H. Schröder, A. Appelhagen, D. Paschek, K. Neymeyer, R. Ludwig
"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"
J. Mol. Liq. **319**, 114207 (2020).
DOI: 10.1016/j.molliq.2020.114207
(12 citations)

83. A. Strate, J. Neumann, T. Niemann, P. Stange, D. Paschek, A.G. Stepanov, A.E. Khudozhitkov, D.I. Kolokolov, R. Ludwig
"Counting cations involved in cationic clusters of hydroxy-functionalized ionic liquids by means of infrared and solid-state NMR spectroscopy"
Phys. Chem. Chem. Phys. **22**, 6861-6867 (2020).
DOI: 10.1039/d0cp00303d
(17 citations)

82. E.A. Shelepova, D. Paschek*, R. Ludwig, N.N. Medvedev
"Comparing the void space and long-range structure of an ionic liquid with a neutral mixture of similar sized molecules"
J. Mol. Liq. **299**, 112121 (2020).
DOI: 10.1016/j.molliq.2019.112121
(9 citations)

2019

81. A.E. Khudozhitkov, V. Overbeck, P. Stange, A. Strate, D. Zaitsau, A. Appelhagen, D. Michalik, A.G. Stepanov, D.I. Kolokolov, D. Paschek, R. Ludwig
"Simultaneous determination of deuteron quadrupole coupling constants and rotational correlation times: the model case of hydrogen bonded ionic liquids"
Phys. Chem. Chem. Phys. **21**, 25597-25605 (2019).
DOI: 10.1039/c9cp04983e
(8 citations)

80. A.E. Khudozhitkov, J. Neumann, T. Niemann, D. Zaitsau, P. Stange, D. Paschek, A. Stepanov, D. Kolokolov, R. Ludwig
"Hydrogen bonding between ions of like charge in ionic liquids characterized by NMR deuteron quadrupole coupling constants - Comparison with salt bridges and molecular systems"
Angew. Chem. Int. Ed. **58**, 17863-17871 (2019).
DOI: 10.1002/anie.201912476
(42 citations)

79. D.H. Zaitsau, J. Neumann, T. Niemann, A. Strate, D. Paschek*, S.P. Verevkin, R. Ludwig
"Isolating the role of hydrogen bonding in hydroxyl-functionalized ionic liquids by means of vaporization enthalpies, infrared spectroscopy and molecular dynamics simulations"
Phys. Chem. Chem. Phys. **21**, 20308-20314 (2019).
DOI: 10.1039/c9cp04337c
(13 citations)

78. T. Niemann, J. Neumann, P. Stange, R. Ludwig, S. Gartner, T.G.A. Young, D. Paschek, G.G. Warr, R. Atkin
"The double-faced nature of hydrogen bonding in hydroxyl-functionalized ionic liquids shown by neutron diffraction and molecular dynamics simulations"
Angew. Chem. Int. Ed. **58**, 12887-12892 (2019).
DOI: 10.1002/anie.201904712
(39 citations)

2018

77. A. Khudozhitkov, P. Stange, A.-M. Bonsa, V. Overbeck, A. Appelhagen, A. Stepanov, D. Kolokolov, D. Paschek, R. Ludwig
"Dynamical heterogeneities in ionic liquids as revealed from deuteron NMR"
Chem. Commun. **54**, 3098-3101 (2018).
DOI: 10.1039/c7cc09440j
(21 citations)

76. A. Strate, V. Overbeck, V. Lehde, J. Neumann, A.-M. Bonsa, T. Niemann, D. Paschek, D. Michalik, R. Ludwig
"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"
Phys. Chem. Chem. Phys. **20**, 5617-5625 (2018).
DOI: 10.1039/C7CP06454C
(24 citations)

75. A. Strate, J. Neumann, V. Overbeck, A.-M. Bonsa, D. Michalik, D. Paschek, R. Ludwig
"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"
J. Chem. Phys. **149** , 193843 (2018).
Special Topic: Chemical Physics of Ionic Liquids
DOI: 10.1063/1.5011804
(20 citations)

74. J. Neumann, B. Golub, L.-M. Odebrecht, R. Ludwig, D. Paschek*
"Revisiting Imidazolium Based Ionic Liquids: Effect of the Conformation Bias of the [NTf2] Anion Studied By Molecular Dynamics Simulations"
J. Chem. Phys. **149** , 193828 (2018).

Special Topic: Chemical Physics of Ionic Liquids
DOI: 10.1063/1.5013096
(41 citations)

2017

73. A.E. Khudozhitkov, P. Stange, B. Golub, D. Paschek, A.G. Stepanov, D.I. Kolokolov, R. Ludwig
"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"
Angew. Chem. Int. Ed. **56**, 14310-14314 (2017).
DOI: 10.1002/anie.201708340
(33 citations)

72. R. Dragomirova, M. Namayandeh-Jorabchi, D. Paschek, S. Wohlrab
"Operational criteria for the separation of alkanes by zeolite membranes"
Chemie Ingenieur Technik **89**, 926-934 (2017).
DOI: 10.1002/cite.201600178
(13 citations)

71. A.-M. Bonsa, D. Paschek, D.H. Zaitsau, V.N. Emel'yaneko, S.P. Verevkin, R. Ludwig
"The relation between vaporization enthalpies and viscosities: Eyring's theory applied to selected ionic liquids"
ChemPhysChem **18**, 1242-1246 (2017).
DOI: 10.1002/cphc.201700138
(10 citations)

70. D. Kerlé, M. Namayandeh-Jorabchi, R. Ludwig, S. Wohlrab, D. Paschek*
"A Simple Guiding Principle for the Temperature Dependence of the Solubility of Light Gases in Imidazolium-based Ionic Liquids Derived from Molecular Simulations"
Phys. Chem. Chem. Phys. **19** , 1770-1780 (2017).
DOI: 10.1039/C6CP06792A
(29 citations)

2016

69. M. Strauch, A.-M. Bonsa, B. Golub, V. Overbeck, D. Michalik, D. Paschek*, R. Ludwig
"Deuteron quadrupole coupling constants and reorientational correlation times in protic ionic liquids"
Phys. Chem. Chem. Phys. **18**, 17788-17794 (2016).
DOI: 10.1039/c6cp01462c
(23 citations)

2015

68. D. Paschek*, B. Golub, R. Ludwig
"Hydrogen Bonding in a Mixture of Protic Ionic Liquids: A Molecular Dynamics Simulation Study"
Phys. Chem. Chem. Phys. **17**, 8431-8440 (2015).
Special Issue: Solvation Science (Bunsen-Tagung Bochum 2015)
DOI: 10.1039/C4CP05432F
(75 citations)

67. K. Fumino, V. Fossog, P. Stange, D. Paschek, R. Hempelmann, R. Ludwig
"Controlling the Subtle Energy Balance in Protic Ionic Liquids: Dispersion Forces Compete with Hydrogen Bonds"
Angew. Chem. Int. Ed. **53**, 2792-2795 (2015).
DOI: 10.1002/anie.201411509
(78 citations)

66. K. Fumino, A.-M. Bonsa, B. Golub, D. Paschek, R. Ludwig
"Non-Ideal Mixing Behavior of Hydrogen Bonding in Mixtures of Protic Ionic Liquids "
ChemPhysChem **16**, 299-304 (2015).
DOI: 10.1002/cphc.201402760
(52 citations)

2014

65. R. Dragomirova, M. Stöhr, C. Hecker, U. Lubenau, D. Paschek, S. Wohlrab
"Desorption-controlled separation of natural gas alkanes by zeolite membranes"
R. Soc. Chem. Adv. **4**, 59831-59834 (2014).
DOI: 10.1039/c4ra13103g
(9 citations)

64. D. Paschek*, R. Ludwig
"Advancing into Water's 'No Man's Land': Two Liquid States?"
Angew. Chem. Int. Ed. **53**, 11699-11701 (2014).
DOI: 10.1002/anie.201408057
(10 citations)

63. K. Neubauer, R. Dragomirova, M. Stöhr, R, Mothes, U. Lubenau, D. Paschek, S. Wohlrab
"Combination of Membrane Separation and Gas Condensation of Advanced Natural Gas Conditioning"
J. Membrane Sci. **453**, 100-107 (2014).
DOI: 10.1016/j.memsci.2013.10.060
(14 citations)

2013

62. K. Neubauer, U. Lubenau, C. Hecker, B. Lücke, D. Paschek, S. Wohlrab
"Abreicherung von Flüssiggas aus Erdgas mittels Zeolithmembranen"
Chemie Ingenieur Technik **85**, 713-722 (2013).
DOI: 10.1002/cite.201200108
(5 citations)

61. D. Kerlé, R. Ludwig, D. Paschek*
"The Influence of Water on the Solubility of Carbon Dioxide in Imidazolium Based Ionic Liquids"
Z. Phys. Chem. **227**, 167-176 (2013).
Special Issue dedicated to Professor Andreas Heintz
DOI: 10.1524/zpch.2013.0344
(15 citations)

2012

60. T. Köddermann, S. Klembt, D. Klasen, D. Paschek, U. Kragl, R. Ludwig
"The Effect of Neutral Ion Aggregate Formation on the Electrical Conductivity of an Ionic Liquid and its Mixtures with Chloroform"
ChemPhysChem **13**, 1748-1752 (2012).
Special Issue: Ionic Liquids
DOI: 10.1002/cphc.201100838
(28 citations)

59. S. Hempel, J. Fischer, D. Paschek, G. Sadowski
"Activity Coefficients of Complex Molecules by Molecular Simulation and Gibbs-Duhem Integration"
Soft Materials **10**, 26-31 (2012).
Special Issue: Molecular Modeling and Simulation in Process and Materials Engineering
DOI: 10.1080/1539445X.2011.599698
(24 citations)

2011

58. D. Paschek*, R. Day, A.E. García,
"Influence of Water-Protein Hydrogen Bonding on the Stability of Trp-Cage Miniprotein. A Comparison Between the TIP3P and TIP4P-Ew Water Models"
Phys. Chem. Chem. Phys. **13**, 19840-19847 (2011).
Themed Issue: The Physics and Chemistry of Water and Ice
DOI: 10.1039/c1cp22110h
(72 citations)

57. Z. Papanyan, C. Roth, D. Paschek, R. Ludwig
"Understanding the Dissolution of Polyols by Ionic Liquids Using the Example of a Well Defined Model Compound"
ChemPhysChem **12**, 2004-2404 (2011).
DOI: 10.1002/cphc.201100437
(22 citations)

56. T. Peppel, C. Roth, D. Paschek, M. Köckerling, R. Ludwig
"The Influence of H-bond Defects on the Properties of Ionic Liquids"
Angew. Chem. Int. Ed. **50**, 6661-6665 (2011); *Angew. Chem.* **123**, 6791-6795 (2011).
DOI: 10.1002/anie.201100199
(111 citations)

55. J. Neuefeind, C. J. Benmore, J. K. R. Weber, D. Paschek
"More Accurate X-ray Scattering Data of Deeply Supercooled Bulk Liquid Water"
Mol. Phys. **109**, 279-288 (2011).
DOI:10.1080/00268976.2010.520040
(38 citations)

54. D. Paschek*, R. Ludwig
"Specific Ion Effects on Water Structure and Dynamics Beyond the First Hydration Shell "
Angew. Chem. Int. Ed. **50**, 352-353 (2011); *Angew. Chem.* **123**, 368-370 (2011).
DOI: 10.1002/anie.201004501
(77 citations)

53. R. Ludwig, D. Paschek
"Cavity Model Challenged: The Hydrated Electron is Localized in Regions of Enhanced Water Density"
ChemPhysChem **12**, 75-77 (2011).
DOI: 10.1002/cphc.201000810
(5 citations)

2010

52. R. Day, D. Paschek, A. E. García
"Microsecond Simulations of the Folding/Unfolding Thermodynamics of the Trp-cage Miniprotein"
Proteins: Structure, Function and Bioinformatics **78**, 1889-1899 (2010).
DOI: 10.1002/prot.22702
(170 citations)

51. D. R. Canchi, D. Paschek, A. E. García
"Equilibrium study of Protein Denaturation by Urea"
J. Am. Chem. Soc. **132**, 2338-2344 (2010).
DOI: 10.1021/ja909348c
(245 citations)

2009

50. H. Conrad, F. Lehmkühler, C. Sternemann, A. Sakko, D. Paschek, L. Simonelli, S. Huotari, O. Feroughi, M. Tolan, K. Hämäläinen
"Tetrahydrofuran Clathrate Hydrate Formation"
Phys. Rev. Lett. **103**, 218301 (2009).
DOI: 10.1103/PhysRevLett.103.218301
(51 citations)

49. D. Paschek*
"How does Solute-Polarization Affect the Hydrophobic Hydration of Methane?"
Z. Phys. Chem. **223**, 1091-1104 (2009).
Special Issue: Water in Chemistry, Biology, and Physics
DOI: 10.1524/zpch.2009.6060
(9 citations)

48. D. Kerlé, R. Ludwig, A. Geiger, D. Paschek*
"Temperature Dependence of the Solubility of Carbon Dioxide in Imidazolium-based Ionic Liquids"
J. Phys. Chem. B **113**, 12727-12735 (2009).
DOI: 10.1021/jp9055285
(103 citations)

47. R. Ludwig, D. Paschek
"Applying the Inductive Effect for Synthesizing Low Melting and Low Viscous Imidazolium-based Ionic Liquids"
ChemPhysChem **10**, 516-519 (2009).
DOI: 10.1002/cphc.200800730
(21 citations)

2008

46. J. Holzmann, R. Ludwig, A. Geiger, D. Paschek
"Temperature and Concentration Effects on the Solvophobic Solvation of Methane in Aqueous Salt Solutions"
ChemPhysChem **9**, 2722-2730 (2008).
Topical Issue: Water at Molecular Interfaces
DOI: 10.1002/cphc.200800544
(13 citations)

45. D. Paschek*, A. Rüppert, A. Geiger
"Thermodynamical and Structural Characterization of the Transformation from a Metastable Low-Density to a Very-High-Density Form of Supercooled TIP4P-Ew Model Water"
ChemPhysChem **9**, 2737-2741 (2008).
Topical Issue: Water at Molecular Interfaces
DOI: 10.1002/cphc.200800539
(55 citations)

44. D. Paschek*, M. Pühse, A. Perez-Goicochea, S. Gnanakaran, A.E. García, R. Winter, A. Geiger
"The Solvent Dependent Shift of the Amide-I Band of a Fully Solvated Peptide in Methanol/Water Mixtures as a Local Probe for the Solvent Composition in the Peptide/Solvent Interface"
ChemPhysChem **9**, 2742-2750 (2008).
Topical Issue: Water at Molecular Interfaces
DOI: 10.1002/cphc.200800540
(14 citations)

43. D. Paschek, S. Hempel, A. E. García
"Computing the Stability Diagram of the Trp-Cage Miniprotein"
Proc. Natl. Acad. Sci. USA **105**, 17754-17759 (2008).
DOI: 10.1073/pnas.0804775105
(144 citations)

42. J. Fischer, D. Paschek, A. Geiger, G. Sadowski
"Addition/Correction: Modeling of Aqueous (Poly Oxyethylene) Solutions: 1. Atomistic Simulations"
J. Phys. Chem. B **112**, 8849-8850 (2008).
DOI: 10.1021/jp8038016
(20 citations)

41. J. Fischer, D. Paschek, A. Geiger, G. Sadowski
"Modeling of Aqueous (Poly Oxyethylene) Solutions: 2. Mesoscale Simulations"
J. Phys. Chem. B **112**, 13561-13571 (2008).
DOI: 10.1021/jp805770q
(50 citations)

40. T. Köddermann, R. Ludwig, D. Paschek
"On the Validity of Stokes-Einstein and Stokes-Einstein-Debye Relations in Ionic Liquids and Ionic Liquids Mixtures"
ChemPhysChem **9**, 1851-1858 (2008).
DOI: 10.1002/cphc.200800102
(145 citations)

39. D. Paschek*, A. Geiger, J. Fischer, G. Sadowski
"Computing Activity Coefficients of Binary Lennard-Jones Mixtures by Gibbs-Duhem Integration"
Z. Phys. Chem. **222**, 687-694 (2008).
DOI: 10.1524/zpch.2008.5319
(7 citations)

38. D. Paschek*, T. Köddermann, R. Ludwig
"The Solvophobic Solvation and Interaction of Small Apolar Particles in Imidazolium-Based Ionic Liquids"
Phys. Rev. Lett. **100**, 115901 (2008).
DOI: 10.1103/PhysRevLett.100.115901
(19 citations)

37. T. Köddermann, R. Ludwig, D. Paschek*
"Ionic Liquids: Dissecting the Enthalpies of Vaporization"
ChemPhysChem **9**, 549-555 (2008).
DOI: 10.1002/cphc.200700814
(119 citations)

36. J. Fischer, D. Paschek, A. Geiger, G. Sadowski
"Modeling of Aqueous (Poly Oxyethylene) Solutions: 1. Atomistic Simulations"
J. Phys. Chem. B **112**, 2388-2398 (2008).
DOI: 10.1021/jp0765345
(85 citations)

35. A. E. García, D. Paschek
"Simulation of the Equilibrium Folding/Unfolding of a Small RNA-Hairpin"
J. Am. Chem. Soc. **130**, 815-817 (2008).
DOI: 10.1021/ja074191i
(122 citations)

2007

34. T. Köddermann, R. Ludwig, D. Paschek
"Molecular Dynamics of Ionic Liquids — A Reliable Description of Structure, Dynamics and Thermodynamics"
ChemPhysChem **8**, 2464-2470 (2007).
DOI: 10.1002/cphc.200700552
(351 citations)

33. J. Holzmann, R. Ludwig, A. Geiger, D. Paschek*
"Pressure and Salt Effects in Simulated Water: Two Sides of the Same Coin?"
Angew. Chem. Int. Ed. **46**, 8907-8911 (2007); *Angew. Chem.* **119**, 9065-9069 (2007).
DOI: 10.1002/anie.200702736
(70 citations)

32. D. Paschek, H. Nymeyer, A. E. García
"Replica Exchange Simulation of Reversible Folding/Unfolding of the Trp-Cage Miniprotein in Explicit Solvent: On the Structure and Possible Role of Internal Water"

J. Struct. Biol. **157**, 524-533 (2007).
Special Issue: Advances in Molecular Dynamics Simulations
DOI: 10.1016/j.jsb.2006.10.031
(111 citations)

2006

31. D. Paschek*, A. Geiger, M. J. Herve, D. Suter
"Adding Salt to an Aqueous Solution of t-Butanol: Is Hydrophobic Association Enhanced or Reduced?"
J. Chem. Phys. **124**, 154508 (2006).
DOI: 10.1063/1.2188398
(20 citations)

30. P. E. Krouskop, J. D. Madura, D. Paschek, A. Krukau
"Solubility of Simple, Non-Polar Compounds in TIP4P-Ew"
J. Chem. Phys. **124**, 016012 (2006).
DOI: 10.1063/1.2138704
(21 citations)

2005

29. D. Paschek*, S. Nonn, A. Geiger
"Low-Temperature and High-Pressure Induced Swelling of a Hydrophobic Polymer-Chain in Aqueous Solution"
Phys. Chem. Chem. Phys. **7**, 2780-2786 (2005).
DOI: 10.1039/b506207a
(34 citations)

28. R. Ludwig, D. Paschek*
"Wasser: Anomalien und Rätsel"
Chemie in unserer Zeit **39**, 164-175 (2005).
DOI: 10.1002/ciuz.200400341
(19 citations)

27. D. Paschek*
"How the Liquid-Liquid Transition Affects Hydrophobic Hydration in Deeply Supercooled Water"
Phys. Rev. Lett. **94**, 217802 (2005).
DOI: 10.1103/PhysRevLett.94.217802
(172 citations)

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Editorial Works

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