Curriculum Vitae

2024/04/25

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Education

- **Dr. rer. nat.:** (summa cum laude) Fakultät Chemie, TU Dortmund, Supervisor: Prof. Dr. Alfons Geiger, Thesis: "Molekulardynamik Simulation der hydrophoben Hydratation nichtionischer Tenside", November 1998.
- **Diploma (Chemistry):** (sehr gut) Fakultät Chemie, TU Dortmund, Supervisor: Prof. Dr. Alfons Geiger, Thesis: "Berechnung von Neutronenstreuspektren aus MD-Simulationsdaten von isotropem (trans-4,4'-n-Pentyl-Cyclohexyl)-Benzonitril (PCH-5)", July 1992.
- **Study (Chemistry):** Fakultät Chemie, TU Dortmund, 1986–1992.

Professional Experience

- **Senior Research Associate:** Universität Rostock, Mathematisch-Naturwissenschaftliche Fakultät, Institut für Chemie, Abteilung Theoretische und Physikalische Chemie, Prof. Dr. Ralf Ludwig, 2010–
- **Senior Research Associate:** Rensselaer Polytechnic Institute, Center for Biotechnology and Interdisciplinary Studies, Department of Physics, Applied Physics, and Astronomy, 110 Eighth Street, Troy, New York 12180-3590 USA. 2008–2010.
- **Researcher:** TU Dortmund, Fakultät Bio- und Chemieingenieurwesen, Lehrstuhl für Thermodynamik, Prof. Dr. Gabriele Sadowski, 2008.
- **Head of DOMUS Young Investigator Research Group:** Leading research group "Molecular Simulations in Biophysics and Chemical Engineering" as part of the modelling and simulation initiative of the TU Dortmund ("DOMUS") (http://www.domus.tu-dortmund.de/). 2006-2008.
- **Visiting Scientist:** Rensselaer Polytechnic Institute, Center for Biotechnology and Interdisciplinary Studies, 110 Eighth Street, Troy, New York 12180-3590 USA, September-October 2005, March 2007.
- **Visiting Scientist:** Los Alamos National Laboratory, Theory Division, Theoretical Biology and Biophysics Group T-10, Los Alamos NM, USA, March-May 2004, September-October 2004.
- **Researcher:** TU Dortmund, Fakultät Chemie, Physikalische Chemie 2a, Prof. Dr. Alfons Geiger, 2001–2008.
- **Post-Doc:** Universiteit van Amsterdam, Faculty of Science, Van 't Hoff Institute for Molecular Sciences, Chair of Chemical Reactor Engineering, Prof. Dr. Rajamani Krishna , 1999–2001.
- **Post-Doc:** TU Dortmund, Fakultät Chemie, Physikalische Chemie 2a, Prof. Dr. Alfons Geiger, 1998–1999.

- **Graduate Researcher:** TU Dortmund, Fakultät Chemie, Physikalische Chemie 2a, Prof. Dr. Alfons Geiger, 1992–1998.
- **Undergraduate Researcher:** TU Dortmund, Fakultät Chemie, Physikalische Chemie 2a, Prof. Dr. Alfons Geiger, 1991–1992.

Teaching Experience

- **Lecture**: Universität Rostock, Bachelor [BA-Che14, 5. Sem. (oblig.)], PC IIIa: "Grundlagen der Statistischen Thermodynamik", Course-No.: 13356 (V: 2 SWS, Ü: 1 SWS); WS 2022/23 (substitute for Prof. B. Corzilius), WS 2018/19, WS 2017/18, WS 2016/17, WS 2015/2016, WS 2014/2015, WS 2013/2014.
- **Lecture:** Universität Rostock, Bachelor [BA-Che14, 6. Sem. (wahloblig.)], PC IV: "Statistische Thermodynamik realer chemischer Systeme CH22", Course-No.: 13372 (V: 2 SWS); SS 2019, SS 2018, SS 2017, SS 2016, SS 2015, SS 2014, SS 2013.
- **Lecture:** Universität Rostock, Master [MA-Che14, 1.-3. Sem. (wahloblig.); MA-Phy18, 2. Sem. (wahloblig.)], PC VIII: "Wasser in den Naturwissenschaften: Struktur, Funktion und Dynamik MCH-W17", Course-No.: 13550 (V: 2 SWS); SS 2020 (with Prof. Dr. R. Ludwig).
- **Lecture:** Universität Rostock, Master [MA-Che10, 1. Sem. (oblig.); MA-Mat10, 1. Sem. (oblig.)], PC VI: "Molekulare Spektroskopie, Molekulardynamische und ab initio-Rechenverfahren", Course-No.: 13381 (V: 2 SWS, Sr.: 2 SWS); WS 2011/12 (with Prof. Dr. R. Ludwig).
- **Lecture:** Universität Rostock, Diplom/Master [D-Che91, 7. Sem. (oblig.); MA-Mat10, 1. Sem. (oblig.)], "Einführung in die Molekulardynamik mit dem Computer", Course-No: 13208 (V: 2 SWS); WS 2010/2011.
- **Laboratory Course:** Universität Rostock, Chemistry, Bachelor [BA-Che14, 3. Sem. (oblig.)], PC II: "Mischphasenthermodynamik und Elektrochemie", Course-No.: 13314, Supervising experiments: "Verdampfungsenthalpie", "Phasenübergang von Schwefelhexafluorid"; WS 2023/24, WS 2022/23, WS 2021/22, WS 2020/21, WS 2019/20.
- **Laboratory Course:** Universität Rostock, Chemistry, Bachelor [BA-Che14, 6. Sem. (oblig.)], PC IIIb: "Statistische Thermodynamik und Transportphänomene", Course-No.: 13356, Supervising experiments: "2.Virialkoeffizient", "DEBYE-Temperatur", "Computersimulation". DP designed experiment "Computersimulation" and re-designed "DEBYE-Temperatur"; SS 2023, SS 2022, SS 2021, SS 2020, SS 2019, SS 2012, SS 2011, SS 2010.
- **Lecture:** TU Dortmund, Chemistry, Master, "Computer Simulation Methods for Biomolecular Simulations"; SS 2005, SS 2007.
- **MD Simulation Course:** TU Dortmund, "Laboratory course on molecular quantum theory and condensed matter simulation" (with Dr. R. Ludwig); SS 2001, SS 2002, SS 2003.
- **Lecture:** TU Dortmund, "Application of Computer Simulation Methods for the Simulation of Complex Molecular Liquids"; SS 1997 (with Prof. Dr. A. Geiger).
- **Teaching Assistant:** TU Dortmund, held weekly seminars supporting general physical chemistry lectures and supervised undergraduate students in practical physical chemistry laboratory courses; WS/SS 1992–1998.

Dissertation

- D. Paschek, "Molekulardynamische Simulation der hydrophoben Hydratation nichtionischer Tenside", Dissertation TU Dortmund 1998, Mainz Verlag Aachen, ISBN 3-89653-522-6.

Reviewer for International Journals

- Journal of the American Chemical Society
- Journal of Physical Chemistry B
- Journal of Physical Chemistry Letters
- Journal of Chemical Physics
- Physical Review E
- Physical Review Letters
- Physica A
- Biophysical Journal
- Journal of Molecular Liquids
- Chemical Physics Letters

Professional Affiliations

- Member of the Board of the European Molecular Liquids Group (EMLG).
- Secretary of the European Molecular Liquids Group (EMLG), 2011-2017.
- Fellow of the International Union of Pure and Applied Chemistry (IUPAC).
- Member of the Deutsche Bunsen-Gesellschaft für Physikalische Chemie (DBG).
- Member of the Gesellschaft deutscher Chemiker (GdCh).
- Member of COST Action CM1206 "EXIL - Exchange on Ionic Liquids", 2015-2017.

Awards

- Poster-Award of the Bunsen-Tagung 2023, "Physical Chemistry of the Energy Transition", June 5-7, 2023, Berlin, Germany, for the Poster *Why Do Liquids Mix? The Effect of Hydrogen Bond Redistribution on the Mixing Behavior of Protic Ionic Liquids*.
- TU Dortmund "Best Dissertation Award" in the Field of Chemistry for the Dissertation *Molecular Dynamics Simulation of the Hydrophobic Hydration of Nonionic Surfactants*. Award Ceremony: February 10, 2000.

Grants and Fellowships

- DOMUS-Fellowship (Dortmunder Forschungsband für Modellbildung und Simulation). Funded Group: "Molecular Simulations in Biophysics and Process Engineering", TU Dortmund, 2006-2008.
- DFG SPP 1155, German Science Foundation Priority Program SPP 1155 "Molecular Modeling and Simulation in Process Engineering" (Project-No.54268623) as "Beteiligte Person", together with Gabriele Sadowski, Lehrstuhl für Thermodynamik, BCI, TU Dortmund, 2007-2010.
- DFG SPP 1191, (Project-No. 187094384) German Science Foundation Priority Program SPP 1191 "Ionic Liquids" as "Antragsteller", together with Ralf Ludwig, Physikalische Chemie, Institut für Chemie, Universität Rostock, 2010-2014.
- DFG SPP 1570, German Science Foundation Priority Program SPP 1570 "Poröse Medien mit definierter Porenstruktur in der Verfahrenstechnik – Modellierung, Anwendungen, Synthese" (Project-No. 206052115) as "Antragsteller", together with Sebastian Wohlrab, Leibniz Institut für Katalyse e.V., 2011-2016.

Software Development

- **MOSCITO:** Toolkit for performing and analyzing molecular dynamics (MD) simulations. Published under the conditions of the General Public License (1997-2024). URL: http://www.moscitomd.org
- **MOSTOOLS:** Collection of tools for performing advanced analysis of molecular dynamics (MD) simulations. Published under the conditions of the General Public License (1997-2024). URL: http://139.30.122.11/paschek/moscito_add.html
- **KMC:** Software for performing kinetic Monte Carlo simulations of particles on discrete lattices. Published under the conditions of the General Public License (1999-2024). URL: http://139.30.122.11/paschek/kmc.html
- **GROMACS:** Incorporated the temperature/density replica exchange molecular dynamics scheme into GROMACS. URLs: http://www.gromacs.org, http://139.30.122.11/paschek/rpmdrun.html
- **MDorado:** A collection of open source Python tools to analyse structural and dynamical properties from molecular dynamics trajectories. Uses FFTs to efficiently compute time correlation functions. URL: https://github.com/Paschek-Lab/MDorado
- **BondAid:** Open source tool to perform the long-time BNP-correction on bond population correlation functions from MD Simulations with cubic periodic boundary conditions URL: https://github.com/Paschek-Lab/BondAid
- **OrthoBoXY:** Introduces a new and simple way to compute true self-diffusion coefficients from MD simulations with periodic boundary conditions without prior knowledge of the viscosity. URL: https://github.com/Paschek-Lab/OrthoBoXY

- **FreeDRelax:** A collection of software tools to compute intramolecular and intermolecular frequency dependent dipolar NMR relaxation rates from MD simulation data. URL: https://github.com/Paschek-Lab/FreeDRelax

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)

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
(2 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

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)

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
(8 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
(15 citations)

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
(11 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)

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)

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
(40 citations)

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)

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)

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
(74 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)

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)

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)

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
(23 citations)

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
(110 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"
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arXiv: 1511.03169 [physics.chem-ph] (2015).
DOI: 10.48550/arXiv.1511.03169

7. D. Paschek, T. Koeddermann, R. Ludwig
"The Solvophobic Solvation and Interaction of Small Apolar Particles in Imidazolium-Based Ionic Liquids is Characterized by Enthalpy-/Entropy-Compensation"
arXiv: 0801.1124 [cond-mat.soft] (2008).
DOI: 10.48550/arXiv.0801.1124

6. D. Paschek, A. Geiger, M.J. Hervé, D. Suter
"Adding Salt to an Aqueous Solution of t-Butanol: Is Hydrophobic Association Enhanced or Reduced?"
arXiv: cond-mat/0507529 [cond-mat.soft] (2006).
DOI: 10.48550/arXiv.cond-mat/0507529

5. D. Paschek, A. Geiger
"Characterizing the stepwise transformation from a low-density to a very-high-density form of supercooled water"
arXiv: cond-mat/0503530 [cond-mat.soft] (2005).
DOI: 10.48550/arXiv.cond-mat/0512199

4. D. Paschek, S. Nonn, A. Geiger
"Low-Temperature and High-Pressure Induced Swelling of a Hydrophobic Polymer-Chain in Aqueous Solution"
arXiv: cond-mat/0512199 [cond-mat.stat-mech] (2005).
DOI: 10.48550/arXiv.cond-mat/0503530

3. D. Paschek
"How the Liquid-Liquid Transition Affects Hydrophobic Hydration in Deeply Supercooled Water"
arXiv: cond-mat/0411724 [cond-mat.stat-mech] (2005).
DOI: 10.48550/arXiv.cond-mat/0411724

2. D. Paschek
"Heat Capacity Effects Associated with the Hydrophobic Hydration and Interaction of Simple Solutes: A Detailed Structural and Energetical Analysis Based on MD Simulations"
arXiv: cond-mat/0402202 [cond-mat.soft] (2004).
DOI: 10.48550/arXiv.cond-mat/0402202

1. D. Paschek
"Temperature Dependence of the Hydrophobic Hydration and Interaction of Simple Solutes: An Examination of Five Popular Water Models"
arXiv: cond-mat/0312252 [cond-mat.soft] (2004).
DOI: 10.48550/arXiv.cond-mat/0312252

Editorial Works

- Co-edited a special issue "Molecular Liquids Meet Ionic Liquids: From Fundamentals to Applications with Particular Attention to Ionic Liquids" of the Journal of Molecular Liquids on the occasion of the 2015 EMLG/JMLG Meeting in Rostock: J. Mol. Liq. **226** (2017) .
- Co-edited a special issue "Water in Chemistry, Biology, and Physics" of Zeitschrift für Physikalische Chemie on the occasion of Alfons Geiger's 65th birthday : Z. Phys. Chem. **223** (Issue 9) (2009) .

Conferences Organized

- **Bunsen-Kolloquium:** "Bridging the Gap between Molecular and Ionic Liquids: Structure, Dynamics, Thermodynamics", Universität Rostock, January 21, 2021. Conference Website.
- **Annual Joint EMLG/JMLG Meeting 2015:** "Molecular Liquids Meet Ionic Liquids From Fundamentals to Applications" Universität Rostock, September 6-10, 2015. Conference Website. Co-organized conference with R. Ludwig.
- **Bunsen-Kolloquium:** "Water in Biology, Chemistry and Physics: Results and Perspectives", TU Dortmund, June 19, 2009. Co-organized conference with R. Ludwig.

Invited Talks

25. D. Paschek "HBPCFs and PBCs: WTF?" Seminar der Theoretischen Chemie der Universität Bonn, October 12, 2023, Mulliken Center für Theoretische Chemie, Universität Bonn, Bonn, Germany.
24. D. Paschek "Short-Time and Long-Time Dynamics of Hydrogen Bonds in Hydroxyl-Funtionalized Ionic Liquids" Joint EMLG/JMLG Meeting 2023 "Understanding Solvation in Molecular and Ionic Fluids: Towards a Sustainable Future", September 4-7, 2023, Bordeaux, France.

23. D. Paschek “Computing the Frequency-Dependent NMR-Relaxation of Phosphonium Ionic Liquids from MD Simulation”, Workshop Arbeitskreis NMR, March 26-29, 2023, Universität Rostock, Rostock, Germany.
22. D. Paschek “Understanding Nonideal Mixing of Protic Ionic Liquids: MD Simulations and Lattice Models” THERMAM 2018, 7th Rostocker International Conference: “Thermophysical Properties for Technical Thermodynamics” July 26-27, 2018, Universität Rostock, Rostock, Germany.
21. D. Paschek “ Nonideal Mixing of Protic Ionic Liquids: The Effect of Hydrogen Bonds”, XXI International Conference on Chemical Thermodynamics in Russia (RCCT-2017) June 26-30, 2017, Nikolaev Institute of Inorganic Chemistry SB RAS, Technopark of Novosibirsk Akademgorodok and Novosibirsk State University, Novosibirsk, Russian Federation.
20. D. Paschek “Denaturierung von Proteinen: Detaillierte Einsicht in die zu Grunde liegenden molekularen Prozesse durch Computersimulationen”, GDCh-Kolloquium, Ernst-Moritz-Arndt Universität Greifswald, June 14, 2012, Greifswald, Germany.
19. D. Paschek “Insights Into the Adsorption of Light Gases in Ionic Liquids from Computer Simulations” Bunsen-Kolloquium “Molecular Thermodynamics of Complex Systems”, Universität Rostock, April 28, 2012, Rostock, Germany.
18. D. Paschek “Computer simulation of the folding/unfolding equilibrium of the Trp-Cage miniprotein: understanding the effects of pressure and denaturants.”, Prague Protein Spring 2012, May 3-6, 2012, Villa Lena, V Sadech 1, 160 00 Prague 6, Czech Republik.
17. D. Paschek “Computer Simulation of Protein Stability: Hydration-, Pressure-, and Co-solvent-Effects”, XVIII International Conference on Chemical Thermodynamics in Russia, RCCT 2011, October 3-7, 2011, Samara, Russian Federation
16. D. Paschek “ Computer Simulation on the Solvation of Hydrophobic Particles and Small Biomolecules in Supercooled Water”, CECAM Workshop “Models for Bulk, Confined Water and Aqueous Solutions Upon Supercooling: State of the Art and Future Perspectives in Understanding Water Anomalies by Computer Simulations”, July 4-7, 2011, CECAM-HQ-EPFL, Lausanne, Switzerland.
15. D. Paschek “Computer Simulation of Protein Stability: Hydration-, Pressure-, and Co-solvent-Effects”, Bunsen-Kolloquium “Water in Chemistry Biology and Physics: Results and Perspectives”, TU Dortmund, June 19, 2009, Dortmund, Germany.
14. D. Paschek “Computer Simulation of the Temperature Dependent Conformational Equilibrium of Small Proteins and Peptides”, International Conference on High-Pressure Molecular Biophysics, December 15, 2008, Synchrotron SOLEIL, L’Orme des Merisier, Saint-Aubain, France.
13. D. Paschek “Using Sampling Enhancement Techniques to Study Solvent Effects on the Folding Equilibrium of Small Proteins with Atomic Detail Simulations”, Kolloquium Department of Chemical Engineering, Imperial College London, December 1, 2008, London, United Kingdom.
12. D. Paschek “Folding proteins under pressure”, Kolloquium der Theoretischen Chemie, Universität Essen, May 8, 2008, Essen, Germany.
11. D. Paschek “Computing properties determining the stability diagram of a miniprotein in dilute aqueous solution by full atomic detail computer simulation”, Symposium “Replica Exchange: New Methods and Applications to Protein Folding and other Large Systems”, The 235th ACS National Meeting, New Orleans, LA, April 6-10, 2008
10. D. Paschek “Berechnung von Löslichkeiten apolarer Moleküle in Wasser und ILs”, Workshop: Perspektiven Physikalische und Theoretische Chemie, February 24-27, 2008, Bad Malente, Germany.
9. D. Paschek “Modeling Water and the Hydrophobic Effect at Extreme Conditions and Calculating Properties Determining the Stability Diagram of a Miniprotein in Aqueous Solutions”, Proteins under Pressure Conference 2008, January 21-25, 2008, Santa Fe, NM, USA.
8. D. Paschek “Computersimulation der reversiblen Temperatur-/Druckinduzierten, Faltung/Entfaltung von Modellpolymeren, Peptiden und kleinen Proteinen” GDCh-Kolloquium, Universität Rostock, December 21, 2006, Rostock, Germany.
7. D. Paschek “Computer Simulation of the Folding/Unfolding Equilibrium of Peptides and Small Proteins”, Colloquium Proteins, Polymers and Water: KU Leuven December 15, Leuven, Belgium 2006
6. D. Paschek “Computer Simulation of the Folding/Unfolding Equilibrium of Peptides and Small Proteins”, Kolloquium des Forschungsbandes “Chemische Biologie und Biotechnologie”, Universität Dortmund, October 16, Dortmund, Germany 2006.

5. D. Paschek "Effect of the hydration water on the folding/unfolding equilibrium of small model proteins" Gordon Research Conference on "Water and Aqueous Solutions" July 30 - August 4, 2006, Holderness School, Plymouth, NH, USA.
4. D. Paschek "Adding Salt to an Aqueous Solution of t-Butanol: Is Hydrophobic Association Enhanced or Reduced?" Pre-GRC Mini-Symposium on Water and Aqueous Solutions, July 29, 2006, Center for Polymer Studies, Boston University, Boston, MA, USA.
3. D. Paschek "The Reversible Temperature-/Pressure Denaturation of Peptides and the Hydrophobic Effect. Large Scale Replica Exchange Molecular Dynamics Simulations" "Chemical Biology across the Frontiers", Chemical Biology Center at Glaxo Smith Kline, March 10-11, 2005 Stevenage, UK.
2. D. Paschek "Die Reversible Temperatur- und Druck-Denataurierung von Peptiden: *Replica Exchange Molecular Dynamics* Simulationen" Kolloquium der Physikalischen Chemie, Universität Rostock, January 19, 2005, Rostock, Germany.
1. D. Paschek "Molecular simulation of hydrophobic interactions in water and aqueous electrolyte solutions", International Bunsen Discussion Meeting "Interfacial Water in Chemistry and Biology", September 19-23, 2003, Velen, Germany.

Contributed Talks and Posters

173. D. Paschek, J. Busch "OrthoBoXY: A Simpler Way to Compute True Self-Diffusion Coefficients and Viscosities from Molecular Simulation" Bunsen-Tagung 2024, "High-Resolution Structural Methods in Material and Life Sciences", March 25-27, 2024, Aachen, Germany (Poster).
172. M. Brandt, E. R. Bensons, B. Corzilius, D. Paschek "Temperature Dependence of the Conformational Landscape of 2-^{13}C-Ethyl-1-^{13}C-Acetate in a Glycerol-Water Environment" Bunsen-Tagung 2024, "High-Resolution Structural Methods in Material and Life Sciences", March 25-27, 2024, Aachen, Germany (Poster).
171. A. M. Chiramel Tony, L. Kruse, A. Strate, R. Ludwig, D. Paschek "A First-Principles Based Approach to Determine the Frequency-Dependent Dipolar ^{19}F-NMR Relaxation in an Ionic Liquid from Molecular Simulation" Bunsen-Tagung 2024, "High-Resolution Structural Methods in Material and Life Sciences", March 25-27, 2024, Aachen, Germany (Poster).
170. F. Freytag, J. K. Philipp, J. Busch, D. Paschek, R. Ludwig "*50 Ways* of Computing the Viscosity of Poly-Ethylene-Glycol Ethers from Molecular Dynamics Simulations" Bunsen-Tagung 2024, "High-Resolution Structural Methods in Material and Life Sciences", March 25-27, 2024, Aachen, Germany (Poster).
169. J. K. Philipp, D. Paschek, R. Ludwig "Structural Diversity of a Pseudo-Ionic Liquid: Investigating Mixtures of [Li][NTf_2] and Triglyme" Bunsen-Tagung 2024, "High-Resolution Structural Methods in Material and Life Sciences", March 25-27, 2024, Aachen, Germany (Talk).
168. R. Ludwig, J. Neumann, D. Paschek, D. Kolokolov "Strengths, distributions and life times of hydrogen bonds in hydroxyl-functionalized ionic liquids" ACS Spring Meeting 2024 "Many Flavours of Chemistry", March 17-21, 2024, New Orleans, LA, USA (Talk).
167. D. Paschek "Combining Frequency Dependent Intermolecular Dipolar NMR Relaxation and MD: Some Advice from Random Walkers and Jack Freed" Workshop Arbeitskreis NMR, March 10-13, 2024, Bad Kissingen, Germany (Talk).
166. D. Paschek "Insights into the Quadrupolar NMR Relaxation of Xenon-131 Dissolved in Supercritical Carbon Dioxide Based on Molecular Dynamics Simulations" Malente Workshop 2024, March 3-6, 2024, Bad Malente, Germany (Talk).
165. A. M. Chiramel Tony, D. Paschek "A First Principles Based Approach to Determine the Frequency-Dependent Dipole-Dipole Relaxation from Molecular Simulations" 11th Meeting of the Graduate Network — Life, Light and Matter 2024, Universität Rostock, January 26, 2024, Rostock, Germany (Talk).
164. M. Brandt, D. Paschek, R. Ludwig "Understanding the Nano-Scale Dynamics of Glycerol-Water Mixtures" Forschungscamp 2023, Universität Rostock, November 23, 2023, Rostock, Germany (Poster).
163. D. Paschek "OrthoBoXY: Computation of True Self-Diffusion Coefficients and Shear Viscosities from MD Simulations Made Easy" Seminar "Moderne Methoden der Physikalischen Chemie zur Untersuchung kondensierter Materie" der Physikalischen Chemie an der Universität Rostock, October 10, 2023, Rostock, Germany (Talk).
162. J. K. Phillip, D. Paschek, R. Ludwig "Pseudo-ionic Liquid and Water-in-salt Electrolyte: Structural Diversity in Mixtures of [Li][NTf_2], Triglyme and Water" EMLG/JMLG Meeting 2023 "Understanding Solvation in Molecular and Ionic Fluids: Towards a Sustainable Future", September 4-7, 2023, Bordeaux, France (Talk).

161. J. Busch, R. Ludwig, D. Paschek "Anisotropic Molecular Reorientation of Methanol Unravelled" EMLG/JMLG Meeting 2023 "Understanding Solvation in Molecular and Ionic Fluids: Towards a Sustainable Future", September 4-7, 2023, Bordeaux, France (Poster).
160. L. Kruse, E. Mock, A. Strate, D. Paschek, D. Rauber, R. Ludwig "Understanding the dynamics of ionic liquids by means of fast-field-cycling NMR relaxometry and molecular dynamics simulations" EMLG/JMLG Meeting 2023 "Understanding Solvation in Molecular and Ionic Fluids: Towards a Sustainable Future", September 4-7, 2023, Bordeaux, France (Poster).
159. L.-E. Christopher, J. Busch, R. Ludwig, D. Paschek "Medium- and Short-Range Structure of $LiNTf_2$-Water-in-Salt-Electrolytes from Molecular Dynamics Simulations" EMLG/JMLG Meeting 2023 "Understanding Solvation in Molecular and Ionic Fluids: Towards a Sustainable Future", September 4-7, 2023, Bordeaux, France (Poster).
158. J. Busch, D. Paschek, T.G.A. Youngs, R. Ludwig "Counting hydrogen bonds in mixtures of ionic liquids and molecular solvents: Geometries, distributions and lifetimes" ACS Fall Meeting 2023 "Harnessing the Power of Data", August 13-17, 2023, San Francisco, CA, USA (Talk).
157. L. Kruse, E. Mock, A. Strate, D. Paschek, D. Rauber, R. Ludwig "Insights into the dynamics of cations and anions in ionic liquids: Combining fast-field-cycling NMR relaxometry and molecular dynamics simulations" ACS Fall Meeting 2023 "Harnessing the Power of Data", August 13-17, 2023, San Francisco, CA, USA (Poster).
156. D. Paschek "Computing Dipolar NMR Relaxation Rates from MD: Some Advice from Interviewing Random Walkers" Seminar "Moderne Methoden der Physikalischen Chemie zur Untersuchung kondensierter Materie" der Physikalischen Chemie an der Universität Rostock, July 14, 2023, Rostock, Germany (Talk).
155. D. Paschek, B. Golub, D. Ondo, R. Ludwig "Why Do Liquids Mix? The Effect of Hydrogen Bond Redistribution on the Mixing Behavior of Protic Ionic Liquids" Bunsen-Tagung 2023, "Physical Chemistry of the Energy Transition", June 5-7, 2023, Berlin, Germany (Poster).
154. S. Fritsch, D. Paschek, R. Ludwig "Improving the Stability of Salty Methane Co-Clathrates with Monovalent Ions as Guests" Bunsen-Tagung 2023, "Physical Chemistry of the Energy Transition", June 5-7, 2023, Berlin, Germany (Poster).
153. J. Busch, D. Paschek, R. Ludwig "Cation-Networks in Hydroxyl-Functionalised Ionic Liquids: Stabilised through Hydrogen Bonds and Challenged by Molecular Solvents" Bunsen-Tagung 2023, "Physical Chemistry of the Energy Transition", June 5-7, 2023, Berlin, Germany (Poster).
152. L. Möhring, J. Busch, D. Paschek, R. Ludwig "Hydrogen Bonded Cations in Carboxy-functionalized Ionic Liquids: A Far-Infrared Spectroscopy Study" Bunsen-Tagung 2023, "Physical Chemistry of the Energy Transition", June 5-7, 2023, Berlin, Germany (Poster).
151. J. Busch, D. Paschek, T.G.A. Youngs, R. Ludwig "How hydrogen bonds in hydroxyl-functionalised ILs stabilise cation- networks and lend a hand to molecular components" Congress on Ionic Liquids COIL-9, April 24-28, 2023, Lyon, France (Talk).
150. D. Paschek "Hydrogen Bond Redistribution Effects in Mixtures of Protic ILs and in Water in Salt IL Systems" Malente Workshop 2023, February 19-22, 2023, Bad Malente, Germany (Talk).
149. J. Busch, D. Paschek, T.G.A. Youngs, R. Ludwig "Hydrogen bonds in hydroxyl-functionalised ionic liquids stabilise cation networks and lend a hand to molecular components" Joint ESS ILL User Meeting, October 5-7, 2022, Lund, Sweden (Poster).
148. D. Paschek "Why Do Liquids Mix? The Effect of Hydrogen Bond Redistribution on the Mixing Behavior of Protic Ionic Liquids" EMLG/JMLG Meeting 2022 "Molecular Liquids at Interfaces", September 12-16, 2022, Barcelona, Spain (Talk).
147. J. Busch, D. Paschek, T.G.A. Youngs, R. Ludwig "When Like-charged Ions Attract: Controlling the Size and Distribution of Cation Clusters in Ionic Liquids by Adding Molecular OH-catchers" EMLG/JMLG Meeting 2022 "Molecular Liquids at Interfaces", September 12-16, 2022, Barcelona, Spain (Talk).
146. J. K. Phillip, D. Paschek, M. Bühl, R. Ludwig "Cluster Formation in Mixtures of [Li][NTf_2] and Triglyme" EMLG/JMLG Meeting 2022 "Molecular Liquids at Interfaces", September 12-16, 2022, Barcelona, Spain (Poster).
145. D. Paschek "Why Do Liquids Mix?" Seminar "Moderne Methoden der Physikalischen Chemie zur Untersuchung kondensierter Materie" der Physikalischen Chemie an der Universität Rostock, July 15, 2022, Rostock, Germany (Talk).
144. D. Paschek "Some Thoughts On Why We Should Try Inventing Compressible Ionic Liquids" Malente Workshop 2022, June 7-10, 2022, Bad Malente, Germany (Talk).

143. D. Paschek, S. Fritsch, J. Busch, J. Neumann "Long-Time Corrections for the Computation of Hydrogen Bond Lifetimes in Water from NVT and NPT Simulations with Cubic and Orthorhombic Periodic Boundary Conditions" Bunsen-Tagung 2022, "Understanding Dispersion Interactions in Molecular Chemistry", June 25-29, 2022, Gießen, Germany (Poster).
142. E. Mock, C. Schröder, R. Ludwig, D. Paschek "Viscosity Based Force Field Evaluation" Bunsen-Tagung 2022, "Understanding Dispersion Interactions in Molecular Chemistry", June 25-29, 2022, Gießen, Germany (Poster).
141. L. Möhring, J. Busch, D. Paschek, R. Ludwig "Doubly Hydrogen Bonded Cation Dimers in Ionic Liquids: A Molecular Dynamics Simulations Study" Bunsen-Tagung 2022, "Understanding Dispersion Interactions in Molecular Chemistry", June 25-29, 2022, Gießen, Germany (Poster).
140. S. Fritsch, D. Paschek, R. Ludwig "Behavior of Salty Methane Co-Clathrates with Monovalent Ions as Guests: An Exploration Based on Molecular Dynamics Simulations" Bunsen-Tagung 2022, "Understanding Dispersion Interactions in Molecular Chemistry", June 25-29, 2022, Gießen, Germany (Talk).
139. J. Busch, D. Paschek, T.G.A. Youngs, R. Ludwig "When Like-Charged Ions Attract: Controlling the Size and Distribution of Cation Clusters in Ionic Liquids by Adding Molecular OH-Catchers" Bunsen-Tagung 2022, "Understanding Dispersion Interactions in Molecular Chemistry", June 25-29, 2022, Gießen, Germany (Talk).
138. E. Mock, C. Schröder, R. Ludwig, D. Paschek "Validation of Polarizable Force Fields Using the Periodic Perturbation Method", "Molecular Simulation 2022: Present, Past and Future", June 25-29, 2022, Erice, Italy (Poster).
137. J. Busch, J. Neumann, D. Paschek, R. Ludwig "Revisiting the Anisotropic Reorientational Motion of Liquid Methanol", "Molecular Simulation 2022: Present, Past and Future", June 25-29, 2022, Erice, Italy (Poster).
136. J. K. Phillip, D. Paschek, M. Bühl, R. Ludwig "Cluster Formation in Mixtures of [Li][NTf_2] and Triglyme" Canada–UK Joint Symposium on Coordination Chemistry, May 30- June 6, 2022, St. Andrews, Scotland (Poster).
135. J. Busch, D. Paschek, T.G.A. Youngs, R. Ludwig "When Like-Charged Ions Attract: Controlling the Size and Distribution of Cation Clusters in Ionic Liquids by Adding Molecular OH-Catchers" Webinar of the European Society of Ionic Matter, "Spectroscopy of Ionic Liquids", March 15-16, 2022 (Talk).
134. D. Paschek "Dynamics and Lifetimes of Hydrogen Bonds in Hydroxyl-Functionalized Ionic Liquids: General Approach,Models and Timescales" Salem Workshop 2021, September 26-29, 2022, Salem, Germany (Talk).
133. S. Fritsch, D. Paschek, R. Ludwig "Do Salty Clathrate Hydrates Exist? — A Theoretical Approach" Bunsen-Tagung 2021 "Multi-Scale Modelling & Physical Chemistry of Colloids" (online), May 10-12, 2021 (Talk).
132. J. Busch, D. Paschek, T.G.A. Youngs, R. Ludwig "When Like-charged Ions Attract: The Influence of Hydroxyl Defects on the Size and Distribution of Cation Clusters in Ionic Liquids" Bunsen-Tagung 2021 "Multi-Scale Modelling & Physical Chemistry of Colloids" (online), May 10-12, 2021 (Talk).
131. D. Paschek "Hydrogen Bond Population Correlation Functions and Periodic Boundary Conditions: Worth the Fuss?" Seminar "Moderne Methoden der Physikalischen Chemie zur Untersuchung kondensierter Materie" der Physikalischen Chemie an der Universität Rostock, April 16, 2021, Rostock, Germany (Talk).
130. J. Busch, T. Niemann, J. Neumann, D. Paschek, R. Ludwig, Särtner, T.G.A. Youngs "When Like-charged Ions Attract: The Influence of Hydroxyl Defects on the Size and Distribution of Cation Clusters in Ionic Liquids" ISIS Student Meeting, October 28-29, 2021 Milton Hill Abingdon, England (Poster).
129. J. Neumann, D. Paschek, R. Ludwig "Hydrogen Bond Dynamics in Ionic Liquids: A Molecular Dynamics Simulation Study" 55th Symposium on Theoretical Chemistry, September 22-29, 2019, Rostock, Germany (Poster).
128. J. Busch, J. Neumann, D. Paschek, R. Ludwig "Studying Hydrogen Bonding in Liquid Methanol by Computing NMR and IR Properties from a Combination of MD Simulations and Ab Initi Calculations" 55th Symposium on Theoretical Chemistry, September 22-29, 2019, Rostock, Germany (Poster).
127. S. Fritsch, D. Paschek, R. Ludwig "Is the Existence of 'Salty Clathrate Hydrates' Possible? - A Theoretical Approach" 55th Symposium on Theoretical Chemistry, September 22-29, 2019, Rostock, Germany (Poster).
126. B. Golub, D. Paschek, R. Ludwig "Hydrogen Bonding in Trialkylammonium Based Protic Ionic Liquids Studied by Molecular Dynamics Simulations" 55th Symposium on Theoretical Chemistry, September 22-29, 2019, Rostock, Germany (Poster).
125. P. Lehmann, B. Golub, D. Paschek, R. Ludwig "Molecular Dynamics Simulations Mixtures of Glycerol with DMSO: Hydrogen Bonds, Structure and Dynamics" 55th Symposium on Theoretical Chemistry, September 22-29, 2019, Rostock, Germany (Poster).

124. J. Busch, J. Neumann, D. Paschek, R. Ludwig "Studying Hydrogen Bonding in Liquid Methanol by Computing NMR and IR Properties from a Combination of MD Simulations and Ab Initi Calculations" EMLG/JMLG Meeting 2019, September 8-12, 2019, Kutná Hora, Czech Republic (Poster).
123. J. Neumann, D. Paschek, R. Ludwig "Hydrogen Bond Dynamics in Ionic Liquids: A Molecular Dynamics Simulation Study" EMLG/JMLG Meeting 2019, September 8-12, 2019, Kutná Hora, Czech Republic (Talk).
122. S. Fritsch, D. Paschek, R. Ludwig "s the Existence of Salty Chlathrate Hydrates Possible? - A Theoretical Approach"" EMLG/JMLG Meeting 2019, September 8-12, 2019, Kutná Hora, Czech Republic (Poster).
121. J. Neumann, D. Paschek, R. Ludwig "Hydrogen Bond Lifetimes in Ionic Liquids: A Molecular Dynamics Simulation Study" Bunsen-Tagung 2019 "Functional Materials", May 30 - June 1, 2019, Jena, Germany (Talk).
120. J. Busch, D. Paschek, R. Ludwig "Computing NMR Properties from a Combination of Molecular Dynamics Simulations and Ab Initio Calculations" Bunsen-Tagung 2019 "Functional Materials", May 30 - June 1, 2019, Jena, Germany (Poster).
119. T. Niemann, J. Neumann, P. Stange, T.G.A. Youngs, D. Paschek, R. Atkin, R. Ludwig "The Double-Faced nature of Hydrogen Bonding in Hydroxyl-Functionalized Ionic Liquids Shown by Neutron Diffraction and Molecular Dynamics Simulations" Bunsen-Tagung 2019 "Functional Materials", May 30 - June 1, 2019, Jena, Germany (Poster).
118. D. Paschek "On The Balance Between Contact and Solvent-Separated Ion-Pairs in Mixtures of the Protic Ionic Liquid Triethylammonium-Methylsulfonate with Water" Malente Workshop 2019, March 10-13, Bad Malente, Germany (Talk).
117. J. Neumann, D. Paschek, R. Ludwig "NMR Quadrupolar Relaxation in Water Revisited: Computing the ^{2}H- and ^{17}O-Relaxation in Liquid and Solid Water from Ab Initio Calculations and Molecular Simulations" EMLG/JMLG Meeting 2018 and and 41st Symposium on Solution Chemistry "Understanding of Molecular Liquids and its Extension to New Fields", November 4-1, 2018, Nagoya, Japan (Talk).
116. D. Paschek "Re-revisiting NMR Quadrupolar Relaxation in Water: Improved Estimation of the ^{2}H- and ^{17}O-Relaxation in Liquid and Solid Water from Ab Initio Calculations and Molecular Simulations " Seminar "Moderne Methoden der Physikalischen Chemie zur Untersuchung kondensierter Materie" der Physikalischen Chemie an der Universität Rostock, June 1, 2018, Rostock, Germany (Talk).
115. D. Paschek, R. Ludwig "Computing NMR Properties from a Combination of Molecular Dynamics Simulations and Ab Initio Calculations" Bunsen-Tagung 2018 "Functional Materials", May 10-12, 2018, Hannover, Germany (Poster).
114. B. Golub, D. Paschek, R. Ludwig "On Polarizable Simulations Using GROMACS: Advances and Challenges" Bunsen-Tagung 2018 "Functional Materials", May 10-12, 2018, Hannover, Germany (Poster).
113. J. Neumann, D. Paschek, R. Ludwig "On Polarizable Simulations Using GROMACS: Advances and Challenges" Bunsen-Tagung 2018 "Functional Materials", May 10-12, 2018, Hannover, Germany (Talk).
112. P. Stange, A.E. Khudozhitkov, D. Kolokolov, D. Paschek, A.G. Stepanov, R. Ludwig "Deuteron Quadrupole Coupling Constants and Dynamical Heterogeneities in Protic Ionic Liquids by Means of Deuteron NMR Spectroscopy" Bunsen-Tagung 2018 "Functional Materials", May 10-12, 2018, Hannover, Germany (Poster).
111. D. Paschek "NMR Quadrupolar Relaxation in Water Revisited: Computing the ^{2}H- and ^{17}O-Relaxation in Liquid and Solid Water from Ab Initio Calculations and Molecular Simulations" Malente Workshop 2018, March 18-21, Bad Malente, Germany (Talk).
110. J. Neumann, D. Paschek, R. Ludwig "Influence of Like-Charged Hydrogen Bonding on the Structure and Dynamics of Ionic Liquids: A Molecular Dynamics Simualtion Study" EMLG/JMLG Meeting 2017, November 10-14, 2017, Vienna, Austria (Poster).
109. B. Golub, D. Paschek, R. Ludwig "Dynamics in Protic Ionic Liquids. What Can We Learn From Different Force Fields?" EMLG/JMLG Meeting 2017, November 10-14, 2017, Vienna, Austria (Talk).
108. B. Golub, D. Paschek, R. Ludwig "Dynamics in Protic Ionic Liquids. What Can We Learn From Different Force Fields?" Bunsen-Tagung 2017 "Physical Chemistry for Life-Sciences", May 25-27, 2017, Kaiserslautern, Germany (Talk).
107. J. Neumann, D. Paschek, R. Ludwig "A Molecular Dynamics Simulation Study of Like-Charged Hydrogen Bonding in Ionic Liquids" Bunsen-Tagung 2017 "Physical Chemistry for Life-Sciences", May 25-27, 2017, Kaiserslautern, Germany (Poster).
106. E. Reiter, D. Paschek, R. Ludwig "Second Osmotic Virial Coefficient for Polar and Nonpolar Solutes in Aqueous Solution from Molecular Simulation" Bunsen-Tagung 2017 "Physical Chemistry for Life-Sciences", May 25-27, 2017, Kaiserslautern, Germany (Poster).

105. D. Paschek "Wasser: Ungewöhnliche Eigenschaften einer scheinbar alltäglichen Substanz" Lange Nacht der Wissenschaften, Universität Rostock, April 27, 2017, Rostock, Germany (Talk).
104. B. Golub, D. Paschek, R. Ludwig "Protic Ionic Liqudis: Polarizable Force Fields" COST CM1206 Meeting, March 3-31, 2017, Lyon, France (Talk).
103. D. Paschek "Protic Ionic Liquids: Understanding Non-Ideal Mixing of Protic Ionic Liquids: Molecular Simulations and Lattice Models" Malente Workshop 2017, March 12-15, Bad Malente, Germany (Talk).
102. B. Golub, D. Paschek, R. Ludwig "Hydrogen Bonding and Mixing Energies in Protic Ionic Liquids" ILWS 2017 Winter School on Ionic Liquids, February 7-10, 2017, Porto, Portugal (Poster).
101. J. Neumann, D. Paschek, R. Ludwig "Like-Charged Hydrogen Bonding in Ionic Liquids" ILWS 2017 Winter School on Ionic Liquids, February 7-10, 2017, Porto, Portugal (Poster).
100. D. Paschek "Solvation-Behavior of Light Gases in ILs: A Simple Guidance Principle Derived from Computer Simulations" Seminar "Moderne Methoden der Physikalischen Chemie zur Untersuchung kondensierter Materie" der Physikalischen Chemie an der Universität Rostock, October 14, 2016, Rostock, Germany (Talk).
99. D. Paschek "Influence of Like-Charged Hydrogen Bonding on the Structure and Dynamics of Ionic Liquids: A Molecular Dynamics Simualtion Study" EMLG/JMLG Meeting 2016 "Progresses on the experimental and theoretical computational techniques for the study of liquid and supercritical fluids: from simple to complex systems", September 11-16, 2016, Platanias-Chania (Crete), Greece (Talk).
98. M. Namayandeh-Jorabchi, D. Kerlé, S. Wohlrab, R. Ludwig, D. Paschek "Solubility Convergence and Criticality in Ionic Liquids" EMLG/JMLG Meeting 2016 "Progresses on the experimental and theoretical computational techniques for the study of liquid and supercritical fluids: from simple to complex systems", September 11-16, 2016, Platanias-Chania (Crete), Greece (Talk).
97. B. Golub, C. Schröder, D. Paschek, R. Ludwig "Dynamics in Mixtures of Protic Ionic Liquids" 26th EUCHEM Conference on Molten Salts and Ionic Liquids, July 3-8, 2016, Vienna, Austria (Poster).
96. J. Neumann, D. Paschek, R. Ludwig "A Molecular Dynamics Simulation Study of Direct Cation-Cation Interactions in Cholinium Based Ionic Liquids" Bunsen-Tagung 2016 "Basic Mechanisms in Energy Conversion", May 5-7, 2016, Rostock, Germany (Poster).
95. B. Golub, C. Schröder, D. Paschek, R. Ludwig "Structure and Dynamics in Mixtures of Protic Ionic Liquids: A Molecular Dynamics Simulation Study" Bunsen-Tagung 2016 "Basic Mechanisms in Energy Conversion", May 5-7, 2016, Rostock, Germany (Poster).
94. M. Namayandeh-Jorabchi, D. Kerlé, S. Wohlrab, R. Ludwig, D. Paschek "Solubility Convergence and Criticality in Ionic Liquids" Bunsen-Tagung 2016 "Basic Mechanisms in Energy Conversion", May 5-7, 2016, Rostock, Germany (Poster).
93. 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 by Means of NMR Relaxation Time Experiments, DFT-Calculations and Molecular Dynamics Simulations"" Bunsen-Tagung 2016 "Basic Mechanisms in Energy Conversion", May 5-7, 2016, Rostock, Germany (Poster).
92. D. Paschek "Computing intermolecular magnetic dipolar relaxation rates from MD simulation: Possible pitfalls" Malente Workshop 2016, March 7-10, Bad Malente, Germany (Talk).
91. E. Reiter, D. Paschek, R. Ludwig "Computing osmotic second virial coeffients of apolar solutes in aqueous solutions" EMLG/JMLG Meeting 2015 "Ionic Liquids Meet Molecular Liquids: From Fundamentals to Applications", September 6-10, 2015, Rostock, Germany (Poster).
90. S. Heckhausen, D. Paschek, R. Ludwig "Predicting the Temperature Dependence of Ice Growth Rates in Supercooled Water Using Molecular Dynamics Simulations" EMLG/JMLG Meeting 2015 "Ionic Liquids Meet Molecular Liquids: From Fundamentals to Applications", September 6-10, 2015, Rostock, Germany (Poster).
89. M. Namayandeh-Jorabchi, S. Wohlrab, D. Paschek "Sorption and Diffusion of Alkanes and Alkenes in Various Ionic Liquids Studied by Molecular Dynamics Simulations" EMLG/JMLG Meeting 2015 "Ionic Liquids Meet Molecular Liquids: From Fundamentals to Applications", September 6-10, 2015, Rostock, Germany (Poster).
88. B. Golub, D. Paschek, R. Ludwig "Hydrogen Bonding in Mixtures of Protic Ionic Liquids Studied by Molecular Dynamics Simulations" EMLG/JMLG Meeting 2015 "Ionic Liquids Meet Molecular Liquids: From Fundamentals to Applications", September 6-10, 2015, Rostock, Germany (Poster).
87. E. Reiter, D. Paschek, R. Ludwig "Computing osmotic second virial coeffients of apolar solutes in aqueous solutions" Bunsen-Tagung 2015 "Solvation Science", May 14-16, 2015, Rostock, Germany (Poster).
86. B. Golub, D. Paschek, R. Ludwig "Hydrogen bonding in mixtures of protic ionic liquids studied by molecular dynamics simulations" Bunsen-Tagung 2015 "Solvation Science", May 14-16, 2015, Rostock, Germany (Poster).

85. M. Namayandeh-Jorabchi, S. Wohlrab, D. Paschek "Sorption and diffusion of alkane/alkene mixtures in ionic liquids studied by molecular dynamics simulations" Bunsen-Tagung 2015 "Solvation Science", May 14-16, 2015, Rostock, Germany (Poster).
84. D. Paschek "Protic Ionic Liquids Describing the Non-Ideal Mixing Behavior of Protic Ionic Liquids" Seminar "Moderne Methoden der Physikalischen Chemie zur Untersuchung kondensierter Materie" der Physikalischen Chemie an der Universität Rostock, April 10, 2015, Rostock, Germany (Talk).
83. D. Paschek "Protic Ionic Liquids Describing the Non-Ideal Mixing Behavior of Protic Ionic Liquids" Malente Workshop 2015, February 15-18, Bad Malente, Germany (Talk).
82. S. Heckhausen, D. Paschek, R. Ludwig "Computational Study of an Antifreeze Protein and its Interactions with Ice and Water " Bunsen-Tagung 2014 "Physical Chemistry on the Nanometer Scale", May 29-31, 2014, Hamburg, Germany (Talk).
81. M. Namayandeh-Jorabchi, D. Paschek, R. Ludwig "Comparing Temperature Dependences of the Solubility of Alkanes and Alkenes in Imidazolium-Based Ionic Liquids" Bunsen-Tagung 2014 "Physical Chemistry on the Nanometer Scale", May 29-31, 2014, Hamburg, Germany (Talk).
80. B. Golub, D. Paschek, R. Ludwig "Comparing Temperature Dependences of the Solubility of Alkanes and Alkenes in Imidazolium-Based Ionic Liquids" Bunsen-Tagung 2014 "Physical Chemistry on the Nanometer Scale", May 29-31, 2014, Hamburg, Germany (Talk).
79. D. Paschek "Computer Simulation of the Adsorption of Alkanes and Alkane-Mixtures in Zeolites" Malente Workshop 2013, March 10-13, 2013, Bad Malente, Germany (Talk).
78. S. Heckhausen, D. Paschek, R. Ludwig "Computer Simulation Study of Molecular Processes in Ice and Supercooled Solutions" EMLG/JMLG Annual Meeting 2012 "Molecular association in fluid phases and at fluid interfaces", September 5-9, 2012, Eger, Hungary (Poster).
77. D. Paschek, K. Fumino, R. Ludwig "Computer Simulation of the OH/D Stretching Band of Liquid Water as a Function of Temperature and Pressure" EMLG/JMLG Annual Meeting 2012 "Molecular association in fluid phases and at fluid interfaces", September 5-9, 2012, Eger, Hungary (Poster).
76. D. Kerlé, D. Paschek, R. Ludwig "Insights into the absorption of light gases in ionic liquids from computer simulations" Bunsen-Tagung 2012 "Ionic Liquids", May 17-30, 2012, Leipzig, Germany (Talk).
75. S. Heckhausen, D. Paschek, R. Ludwig "Molecular dynamics simulations of the growth of hexagonal ice in supercooled water" Bunsen-Tagung 2012 "Ionic Liquids", May 17-30, 2012, Leipzig, Germany (Talk).
74. D. Paschek, K. Neubauer, S. Wohlrab "Adsorption of alkane-mixtures in zeolite membranes" Bunsen-Tagung 2012 "Ionic Liquids", May 17-30, 2012, Leipzig, Germany (Poster).
73. D. Kerlé, T. K"oddermann, D. Paschek, R. Ludwig "The influence of water on the structure and dynamics of ionic liquids" Bunsen-Tagung 2012 "Ionic Liquids", May 17-30, 2012, Leipzig, Germany (Poster).
72. D. Paschek "Computing the OH-/OD-Stretch Band of Liquid Water as a Function of Temperature (and Pressure)" Seminar "Moderne Methoden der Physikalischen Chemie zur Untersuchung kondensierter Materie" der Physikalischen Chemie an der Universität Rostock, May 25, 2012, Rostock, Germany (Talk).
71. D. Paschek "Computer Simulation of the Adsorption of Alkanes and Alkane-Mixtures in Zeolites" Malente Workshop 2012, February 26-29, 2012, Bad Malente, Germany (Talk).
70. D. Paschek, D. Kerlé, R. Ludwig "Insights Into the Adsorption of Light Gases in Ionic Liquids from Computer Simulations" Fall Meeting DFG SPP 1191 "Ionic Liquids" November 28-30, 2011, Fürth, Germany (Talk).
69. D. Paschek, R. Giernoth, R. Ludwig "Computing the intermolecular magnetic dipole-dipole cross-relaxation in Ionic Liquids", Fall Meeting DFG SPP 1191 "Ionic Liquids" November 28-30, 2011, Fürth, Germany (Poster).
68. D. Paschek "The Liquid-Liquid Phase Transition: Consequences for Hydrophobic Interaction and Protein Stability" EMLG/JMLG Annual Meeting 2011 "New outlook on molecular liquids from short scale to long scale dynamics", September 11-15, 2011, Warsaw, Poland (Talk).
67. S. Heckhausen, J. Holzmann, D. Paschek, R. Ludwig "Simulation of Ice and Cryoprotectant Solutions:Structure and Dynamics" EMLG/JMLG Annual Meeting 2011 "New outlook on molecular liquids from short scale to long scale dynamics", September 11-15, 2011, Warsaw, Poland (Poster).
66. K. Wittler, D. Paschek, R. Ludwig "Water fluctuations in the hydration shell of a 13-mer DNA duplex", Bunsen-Tagung 2011 "Analysis and Control of Ultrafast Photoinduced Reactions", June 2-4, 2011, Berlin, Germany (Poster).
65. D. Paschek, R. Giernoth, R. Ludwig "How structure and dynamics affect the intermolecular magnetic dipole-dipole cross-relaxation in Ionic Liquids", Bunsen-Tagung 2011 "Analysis and Control of Ultrafast Photoinduced Reactions", June 2-4, 2011, Berlin, Germany (Poster).

64. D. Paschek, R. Ludwig "Effect of Ionicity on the Intermolecular Magnetic Dipole-Dipole Cross-Relaxation in Ionic Liquids", Meeting DFG SPP 1191 "Ionic Liquids" March 31, 2011, Potsdam, Germany (Talk).
63. D. Paschek "Simulation of the Trp-Cage Miniprotein: Force Field Issues and the Influence of the Water Model" Malente Workshop 2011, March 20-23, 2011, Bad Malente, Germany (Talk).
62. D. Paschek, D.R. Canchi, A.E. García "An Equilibrium Study of Urea Denaturation of Trp-Cage Miniprotein", EMLG/JMLG Annual Meeting 2010 "Complex Liquids: Modern trends in exploration, understanding and application", September 5-9, 2010, Lviv, Ukraine (Talk).
61. D. Kerlé, D. Paschek, R. Ludwig "Understanding the solubility of gases in ionic liquids from molecular simulations", EMLG/JMLG Annual Meeting 2010 "Complex Liquids: Modern trends in exploration, understanding and application", September 5-9, 2010, Lviv, Ukraine (Talk).
60. S. Heckhausen, J. Holzmann, R. Ludwig, D. Paschek "Effects of cryoprotectants on the hydrophobic hydration of small apolar solutes in aqueous solutions", EMLG/JMLG Annual Meeting 2010 "Complex Liquids: Modern trends in exploration, understanding and application", September 5-9, 2010, Lviv, Ukraine (Poster).
59. J. Holzmann, D. Paschek, R. Ludwig "Dynamics of water in aqueous salt solutions", EMLG/JMLG Annual Meeting 2010 "Complex Liquids: Modern trends in exploration, understanding and application", September 5-9, 2010, Lviv, Ukraine (Poster).
58. D. Paschek "Computer Simulation of Protein Stability", Kolloquium des Instituts für Chemie der Universität Rostock, July 15, 2010, Rostock, Germany (Talk).
57. D. Paschek, R. Ludwig "Predicting frequency dependent cross relaxation rates from Molecular Dynamics Simulations to provide a basis for a reliable interpretation of experimental NOE data", June 17-18, 2010, DFG SPP 1191 "Ionic Liquids" meeting 2010, Berlin, Gremany (Talk).
56. D. Paschek "Predicting frequency dependent cross relaxation rates from Molecular Dynamics Simulations to provide a basis for a reliable interpretation of experimental NOE data" DFG Antragskolloquium SPP 1191, May 26-27, 2010, Potsdam, Germany (Talk).
55. D. Paschek "An Equilibrium Study of Urea Denaturation of Trp-Cage Miniprotein", Bunsen-Tagung 2010 "Interfacial Systems Chemistry: Out of the Vacuum, Through the Liquid, Into the Cell", May 13-15, 2010, Bielefeld, Germany (Talk).
54. A.E. García, D.R. Canchi, C.A. Jiminez, D. Paschek "Microsecond simulations of the detailed folding/unfolding thermodynamics of proteins under various solvent conditions" Symposium: "Generalized-Ensemble Simulation Methods: Symposium in Honor of Dr. Bernd Berg's 60th Birthday", The 239th ACS National Meeting, March 21-25, 2010, San Francisco, California (Talk)
53. D. Paschek "Protein Denaturation by Urea Novel lnsights Provided by Atomic DetailMolecular Simulations " Malente Workshop 2010, February 14-17, 2010, Bad Malente, Germany (Talk).
52. D. Kerlé, D. Paschek, R. Ludwig "Solubility of Carbon Dioxide in Imidazolium-based Ionic Liquids by Molecular Dynamics Simulations", EMLG/JMLG Annual Meeting "Intermolecular Interactions and Liquid Structure", September 6-10, 2009, Salzburg, Austria (Talk).
51. A.E. García, R. Day, N. Sgourakis, D. Paschek "Comparison of the computed folding thermodynamics of Trp-cage miniprotein under various force fields and water models", Symposium "Progress in Polarizable Force Fields and Simulation", The 237th ACS National Meeting, Salt Lake City, UT, March 22-26, 2009 (Talk)
50. J. Holzmann, R. Ludwig, D. Paschek "Structure and dynamics of aqueous salt solutions: An MD simulation study on the influence of different salts", 15th International Conference on the Properties of Water and Steam, September 7-11, 2008, Berlin, Germany (Talk).
49. J. Fischer, S. Hempel, D. Paschek, G. Sadowski "Bestimmung von Aktivitätskoeffizienten assoziierender Moleküle in wässrigen Lösungen durch MD-Simulation und Gibbs-Duhem-Integration", Thermodynamik-Kolloquium/Ingenieurdaten tdy08 , September 24-26, 2008, Erlangen-Nürnberg, Germany (Talk).
48. D. Paschek, "Calculating the Stability Diagram of the Trp-Cage Miniprotein from Atomic Detail Computer Simulations in an Explicit Solvent", "Simulation of Cold Denaturation of Small Proteins", Workshop DFG Forschergruppe 436 , July 8, 2008, Witten-Bommerholz, Germany (Talk).
47. J. Holzmann, R. Ludwig, D. Paschek "Structure and dynamics of aqueous salt solutions: An MD simulation study on the influence of different salts", Bunsen-Tagung 2008, May 1-3, 2008, Saarbrücken, Germany (Talk).
46. J. Fischer, J. Caßens, D. Paschek, G. Sadowski "Activity coefficients of associating fluids in aqueous solution by molecular dynamics simulation" International Workshop Molecular Modeling and Simulation in Applied Material Science, March 10-11, 2008, DECHEMA, Frankfurt, Germany (Talk).

45. A.E. García, S. Yang, D. Paschek, J.N. Onuchic, H. Levine "Use of coarse-grained Langevin dynamics to extract folding times from replica exchange simulations", Symposium "Multiscale Modeling in Biophysics", The 235th ACS National Meeting, New Orleans, LA, April 6-10, 2008 (Talk).
44. A.E. García, D. Paschek "Calculation of the folding/unfolding thermodynamics of an RNA tetraloop by replica exchange molecular dynamics", Symposium "Replica Exchange: New Methods and Applications to Protein Folding and other Large Systems", The 235th ACS National Meeting, New Orleans, LA, April 6-10, 2008 (Talk).
43. A.E. García, Ryan Day, Dietmar Paschek "Theoretical dtudies of pressure effects on folding/unfolding of proteins and nuclei acids", Symposium "Structural Determination, Refinement, and Modeling of Large Biomolecular Complexes", The 234th ACS National Meeting, Boston, MA, August 19-23, 2007 (Talk).
42. A. E. García, D. Paschek "Simulation of the Equilibrium Folding/Unfolding of a Small RNA-Hairpin" *European Biophysics Congress*, Imperial College London, 14th-19th July 2007 (Poster).
41. J. Holzmann, D. Paschek, R. Ludwig " Pressure and salt effects in simulated water: Two sides of the same coin?", Bunsen-Tagung 2007, May 17-19, 2007, Graz, Austria (Poster).
40. R. R. Burri, D. Paschek, A. Geiger "REMD Simulation of Abeta16-22 aggregation in explicit solvent", CSB07 Workshop "From Computational Biophysics to Systems Biology, Forschungszentrum Jülich, 2-4 May 2007 (Poster).
39. S. Gnanakaran, D. Paschek, S. M. Decatur, A.E. García, R. M. Hochstrasser "Connecting the wiggling and jiggling of atoms to measurements: Capturing differences in local solvent structure around peptides", Symposium "Vibrational Spectroscopy as a Probe of Biomolecular Structure and Dynamics: Theory and Experiment", The 233rd ACS National Meeting, Chicago, IL, March 25-29, 2007 (Talk).
38. D. Paschek "Simulation of Cold Denaturation of Small Proteins", Kolloquium DFG Forschergruppe 436 , February 20, 2007, Witten-Bommerholz, Germany (Talk).
37. J. Fischer, G. Sadowski, D. Paschek, A. Geiger "Coarse-graining of effective potentials by iterative Boltzmann-inversion", Industrial Fluid Properties Simulation Collective Workshop, September 18-19, 2006 St. Paul, MS, USA, 2006 (Poster).
36. D. Paschek "Characterizing the stepwise transformation from a low density to a very high density form of supercooled liquid water", Bunsen-Tagung 2006, May 25-27, 2006, Erlangen, Germany (Talk).
35. D. Paschek "Replica Exchange Simulation of the Folding/Unfolding Equilibrium of the Trp-cage Miniprotein in an Explicit Solvent" Bunsen-Tagung 2006, May 25-27, 2006, Erlangen, Germany (Poster).
34. D. Paschek "Replica Exchange Simulation of the Folding/Unfolding Equilibrium of the Trp-cage Miniprotein in an Explicit Solvent" 367. WE-Heraeus-Seminar: "Biomolecular Simulation: From Physical Principles to Biological Function" May 22-24, 2006, Bad Honnef, Germany (Poster).
33. R. Burri, D. Paschek, A Geiger "Aggregation of Amyloid-β peptides (Aβ-22) in aqueous solution observed in Molecular Dynamics simulations" 367. WE-Heraeus-Seminar: "Biomolecular Simulation: From Physical Principles to Biological Function" May 22-24, 2006, Bad Honnef, Germany (Poster).
32. D. Paschek "Replica Exchange Simulation of the Folding/Unfolding Equilibrium of the Trp-cage Miniprotein in an Explicit Solvent", Hünfeld Workshop on "Computersimulation and the Theory of Macromolecules 2006", May 19-20, 2006, Hünfeld, Germany (Talk).
31. D. Paschek "Workshop: Einführung in die Simulation einfacher molekularer Systeme" Universität Rostock, January 20, 2006, Rostock, Germany (Talk).
30. D. Paschek "Computersimulation des Faltungs-/Entfaltungsgleichgewichtes von Proteinen", Kolloquium des Forschungsbandes "Modellbildung und Simulation" Universität Dortmund, December 12, 2005, Dortmund, Germany (Talk).
29. N.N. Medvedev, A.V. Anikeenko, M.G. Anlinchenko, V.P. Voloshin, D. Paschek, A. Appelhagen, A. Geiger "Application of Voronoi Diagrams for Calculation of the Radial Correlation of the Intermolecular Voids" Second International Symposium on Voronoi Diagrams in Science and Engineering, Hanyang University, Seoul, Korea October 10-13, 2005 (Talk).
28. D. Paschek, A.E. García "Reversible temperature and pressure denaturation of protein fragments: Replica exchange molecular dynamics simulation studies" Biomolecular Simulation Congress 2005, Bordeaux, France, September 2-3, 2005 (Poster).
27. D. Paschek, A.E. García "Reversible temperature and pressure denaturation of protein fragments: Replica exchange molecular dynamics simulation studies" 6th Liquid Matter Conference, Utrecht, The Netherlands, July 2-6, 2005 (Poster).

26. D. Paschek "Simulation of the Reversible Temperature and Pressure Denaturation of Small Peptides" Workshop der DFG-Forschergruppe 436, Universität Rostock, April 5-7, 2005, Rostock, Germany (Talk).
25. D. Paschek "Die Reversible Temperatur- und Druck-Denaturierung von Peptiden und der hydrophobe Effekt: Einsichten in molekulare Prozesse durch massiv parallele *Replica Exchange Molecular Dynamics* Simulationen" Kolloquium des Forschungsbandes "Molekulare Aspekte der der Biowissenschaften/Biologisch-chemische Mikrostrukturtechnik" der Universität Dortmund January 18, 2005, Dortmund, Germany (Talk).
24. D. Paschek "Adding Salt to an Aqueous Solution of Tertiary Butanol: Do We Observe a Hydrophobic Effect?", Workshop Graduiertenkolleg "Struktur-Dynamik Beziehungen in mikrostrukturierten Systemen", December 14, 2004, Witten, Germany (Talk).
23. D. Paschek "Heat Capacity Effects Associated with Hydrophobic Hydration", Gordon Research Conference "Water and Aqueous Solutions", August 1-6, 2004 Plymouth, NH, USA (Poster).
22. D. Paschek, A. E. García "Reversible temperature and pressure denaturation of a protein fragment: A replica exchange molecular dynamics simulation study ", Gordon Research Conference "Water and Aqueous Solutions", August 1-6, 2004 Plymouth, NH, USA (Poster).
21. D. Paschek "Hydrophobe Effekte und Wechselwirkungen in reinem Wasser und wässrigen Elektrolytlösungen" Bunsen-Tagung 2004, May 20-22, 2004, Dresden, Germany (Talk).
20. D. Paschek "Hydrophobic Hydration and Hydrophobic Interactions", International Bunsen Discussion Meeting "Interfacial Water in Chemistry and Biology", September 19-23, 2003, Velen, Germany (Poster).
19. D. Paschek, A. Krukau, A. Geiger "Temperaure-dependncent Conformations of a Small Elastin-like Peptide", International Bunsen Discussion Meeting "Interfacial Water in Chemistry and Biology", September 19-23, 2003, Velen, Germany (Poster).
18. D. Paschek "Salt Effects on Hydrophobic Hydration and Interaction" Workshop DFG Forschergruppe 436, TU Darmstadt, March 20-22, 2003, Darmstadt, Germay (Talk).
17. I. Brovchenko, A. Oleinikova, A. Geiger, D. Paschek, "Phase coexistence and dynamic properties of water in nanopores", 2nd International Workshop of Water in Confinement, January 22-25, 2003, Grenoble, France. (Poster).
16. D. Paschek, R. Krishna "Monte Carlo simulation of isobutane adsorbed in silicalite", 13th International Zeolite Conference, July 8-13, 2001, Montpellier, France. (Poster).
15. D. Paschek "Computing the NMR relaxation of ^{131}Xenon in supercritical carbon dioxide" Computational Chemistry Seminar, Universiteit van Amsterdam, Amsterdam, The Netherlands, January 23rd, 2001
14. I. Brovchenko, A. Geiger, D. Paschek "Simulation of water confined in pores in equilibrium with a bulk reservoir" 4th International Congress of Chemical and Process Engineering, August 27-31 August 2000, Praha, Czech Republic. (Poster).
13. Ivan Brovchenko, Dietmar Paschek and Alfons Geiger "Gibbs ensemble simulation of water in spherical cavities", International Bunsen Discussion Meeting "Metastable Water", Nordkirchen, Germany, September 22-26, 1999 (Poster).
12. D. Paschek, T. Engels, W. v. Rybinski and A. Geiger "Hydrophobic aggregation of nonionic surfactants in aqueous solution: An MD simulation study", Technical University Hamburg-Harburg (TUHH), Hamburg, Germany, May 27, 1999 (Talk).
11. D. Paschek, T. Engels, W. v. Rybinski and A. Geiger "MD Simulation der hydrophoben Wechselwirkung nichtionischer Tenside", Seminar "Probleme aus Physik und Chemie der kondensierten Materie", December 10, 1998, Universität Dortmund, Dortmund , Germany (Talk).
10. D. Paschek, T. Engels, W. v. Rybinski and A. Geiger "Hydrophobic interactions of nonionic surfactants", Euroconference "Dynamics of Complex molecular Systems — Computer Simulations and Experiments", May 24–28, 1998, Vaals, The Netherlands. (Poster)
9. D. Paschek, A. Geiger "Simulation of liquid crystals using realistic potentials", Mini–Symposium "Freestanding Smectic Films", July 17–18, 1997, Paderborn, Germany (Talk).
8. D. Paschek, S. Y. Yakovenko, A. A. Muravski A. Geiger "Atomistic modelling of ferroelectric liquid crystals", 6'th International Conference on Ferroelectric Liquid Crystals, July 8–10, 1997, Brest, France. (Talk).
7. D. Paschek, A. Geiger "Molecular dynamics of supercooled water" Bunsen-Tagung 1997, May 8–10, 1997, Darmstadt (Poster).
6. D. Paschek, F. Eikelschulte, A. Geiger "Realistic potentials for the simulation of liquid crystalline compounds" 11'th Molecular Modelling Workshop 1997, May 6–7, 1997, Darmstadt, Germany (Poster).

5. D. Paschek, A. Geiger "Molecular dynamics of ST2 water in the supercooled range", C.N.R.S and DFG Joint Meeting "Elementary Dynamics Processes in Liquids", November 27–30, 1995, Vaals, The Netherlands (Talk).
4. D. Paschek, A. Geiger, "Molecular Dynamics of Supercooled Water", Meeting der European Molecular Liquids Group (EMLG) 2015, European Science Foundation Conference "Molecular Liquids", September 22–27, 1995, Blankenberge, Belgium (Poster).
3. D. Paschek, A. Geiger, "Molecular dynamics simulations of small polar molecules on oxide surfaces" Bunsen-Tagung 1995, May 25–27, 1995, Bremen, Germay (Poster).
2. D. Paschek, A. Geiger, "Molecular dynamics simulations of ammonia adsorbed on titanium dioxide (Rutile) surfaces", 1st European Conference on Computational Chemistry (E.C.C.C.1), May 22–26, 1994, Nancy, France (Poster).
1. R. Niepmann, D. Paschek, A. Geiger, B. Boddenberg, "Untersuchungen zur Dynamik von adsorbierten Ammoniak–Molekülen auf Titan–Dioxid (Rutil) Oberflächen", Bunsen-Tagung 1994, May 12–14, 1994, Berlin, Germany (Poster).