Prof. Dr. Ralf Ludwig

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Physikalische und Theoretische Chemie
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Education

1980	Abitur, Heisenberg-Gymnasium, Gladbeck, Germany
1988	Diploma in Physics, RWTH Aachen, Germany
1991	Dr. rer. nat., Physical Chemistry, RWTH Aachen

Professional experience

1991-1993	Postdoctoral Fellow, RWTH Aachen, Germany
1993-1995	Research Fellow, University of Wisconsin, Madison, USA
1995-1999	Scientific Assistant (C1), University of Dortmund, Germany
1999	Habilitation in Physical Chemistry, University of Dortmund, Germany
2000-2004	Assistant Professor (C2), Physical Chemistry, University of Dortmund, Germany
2004	Visiting Professor, Université Louis Pasteur, Strasbourg, France
2004-2012	Professor (C3), Physical and Theoretical Chemistry, University of Rostock, Germany
2006-2010	Member of the Teaching Commission of the Bunsen (German Physical Chemistry) Society
2006-2010	Executive Director of the Chemistry Department at the University of Rostock, Germany
since 2007	Associated Professor and Divisional Head at the Leibniz-Institute for Catalysis e.V. (LIKAT) at the University of Rostock, Germany
since 2007	Board Member of the Department „Life, Light and Matter“ of the Interdisciplinary Faculty at the University of Rostock, Germany
2007	Vice Dean of the Faculty of Mathematics and Natural Sciences
since 2009	Editorial Board Member „Zeitschrift für Physikalische Chemie“
2011	Chair (W3), Physical Chemistry, University of Freiburg, Germany, declined
since 2012	Chair (W3), General Physical and Theoretical Chemistry, University of Rostock, Germany
since 2012	Head of Physical Chemistry, University of Rostock, Germany
2012-2014	Project director of “Nano4Hydrogen” at the University of Rostock, Germany
since 2014	Regional officer for the state of Mecklenburg-Vorpommern in the Project HYPOS (Hydrogen Power East Germany), BMBF, Germany
since 2017	Editorial Board Member “Scientific Reports”, Nature Publishing Group

2018 Visiting professor at the University of Lille, France

Positions in Scientific Organizations

2016-2020 Elected Member, DFG Review Board “Physical and Theoretical Chemistry”
2016-2021 Elected Member, Board of the Bunsen (German Physical Chemistry) Society
2017 Evaluation Board Member, Chemistry Faculty, University Duisburg-Essen
2017 Member of the Review Panel “C11 – Natural Sciences” within the German Excellence Strategy
since 2018 Chair of the General Meeting of the Leibniz-Institute for Catalysis (LIKAT)
since 2018 Member of the DFG-NFDI Expert Committee
2019-2021 Chair of the German University Professors in Chemistry (ADUC)
since 2019 Chair of the European Molecular Liquids Group (EMLG)
since 2020 Elected Member of the DFG Senate
since 2023 Chair of the Bunsen (German Physical Chemistry) Society

Selected Synergistic Activities and Honours

1993-1995 Grant of Heinrich-Hertz-Stiftung, North Rhine-Westphalia
1996-2000 Best researcher award of the state of North Rhine-Westphalia, Germany
2009 Organizer (with R. Winter) of the International Bunsen Discussion Meeting on "Water in Biology, Chemistry and Physics: Results and Perspectives", Dortmund, Germany
2011 Organizer (with D. Paschek) of the Bunsenkolloquium "Molecular Thermodynamics of Complex Systems", Rostock, Germany
2015 Organizer (with D. Paschek) of the EMLG/JMLG-Meeting “Molecular Liquids meet Ionic Liquids – From Fundamentals to Applications”, Rostock, Germany
2016 Organizer of the 115th General Assembly of the German Bunsen Society for Physical Chemistry, Rostock, Germany
2019 Organizer (with O. Kühn) of the 55th Symposium on Theoretical Chemistry (STC) “Spectroscopy and Photoinduced Dynamics”, Rostock, Germany
2021 Organizer (with M. Brasholz, W. Seidel) of the first virtuell Chemiedozententagung, Rostock, Germany
2023 Organizer of the AK NMR meeting, Rostock, Germany

Current Research Interests

Anomalies, Structure, and Dynamics of Water and Aqueous Solutions; Properties of Ionic Liquids, Hydrogen-Bonded Networks, Hydration of Ions, Bio- and Organic Molecules, Hydrophobic Effects, Influence of Temperature, Pressure, and Additives on the Aggregation Behaviour of Organic Molecules and on the Structure of Biomolecules, Mechanistic Understanding of Catalytic Reactions, Prediction of Macroscopic Properties on the Basis of Molecular Interactions

Publications and Scientific Lectures

About 310 full (peer reviewed) papers and 100 invited lectures (**WoS h-index 65**)

Selected Research Contributions (10 most-cited publications)

[1] R. Ludwig, Water: From Clusters to the Bulk, *Angew. Chem.* **2001**, 113, 1856-76; *Angew. Chem. Int. Ed.* **2001**, 40, 1808-27. (Times cited: 1147)

[2] A. Boddien, D. Mellmann, F. Gärtner, R. Jackstell, H. Junge, P. J. Dyson, G. Laurenczy, R. Ludwig, M. Beller, Efficient Dehydrogenation of Formic Acid Using an Iron Catalyst, *Science* **2011**, 33, 1733-36. (Times cited: 683)

[3] K. Fumino, A. Wulf, R. Ludwig, Strong, Localized, and Directional Hydrogen Bonds Fluidize Ionic Liquids, *Angew. Chem. Int. Ed.* **2008**, 47, 8731-34. (Times cited: 363)

[4] T. Köddermann, D. Paschek, R. Ludwig, Molecular Dynamics Simulations of Ionic Liquids: A Reliable Description of Structure, Thermodynamics and Dynamics, *ChemPhysChem* **2007**, 8, 2464-70. (Times cited: 344)

[5] T. Köddermann, C. Wertz, A. Heintz, R. Ludwig, Ion-Pair Formation in the Ionic Liquid 1-Ethyl-3-methylimidazolium-bis(triflyl)imide as a Function of Temperature and Concentration, *ChemPhysChem* **2006**, 7, 1944-49. (Times cited: 290)

[6] T. Köddermann, C. Wertz, A. Heintz, R. Ludwig, The Association of Water in Ionic Liquids: A Reliable Measure of Polarity, *Angew. Chem. Int. Ed.* **2006**, 45, 3697-3702. (Times cited: 264)

[7] K. Fumino, A. Wulf, R. Ludwig, Hydrogen Bonding in Protic Ionic Liquids: Reminiscent of Water, *Angew. Chem. Int. Ed.* **2009**, 48, 3184-86. (Times cited: 276)

[8] K. Fumino, A. Wulf, R. Ludwig, The Cation-Anion Interaction in Ionic Liquids Probed by Far Infrared Spectroscopy, *Angew. Chem. Int. Ed.* **2008**, 47, 3830-34. (Times cited: 230)

[9] K. Fumino, T. Peppel, M. Geppert-Rybczynska, D. H. Zaitsau, J. K. Lehmann, S. P. Verevkin, M. Köckerling, R. Ludwig, The Influence of Hydrogen Bonding on the Physical Properties of Ionic Liquids. *Phys. Chem. Chem. Phys.* **2011**, 13, 14064-75. (Times cited: 254)

[10] A. Wulf, K. Fumino, R. Ludwig, Spectroscopic Evidence for an Enhanced Anion-Cation Interaction from Hydrogen Bonding in Pure Imidazolium Ionic Liquids, *Angew. Chem.* **2010**, 122, 459-463. *Angew. Chem. Int. Ed.* **2010**, 49, 449-53. (Times cited: 223)

Selected Research Contributions (last three years 2023-20)

[1] 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.* **2023**, 14, 17, 4019–4025.

[2] J. Busch, D. Kotwica, L. Al Sheakh, 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.* **2023**, 14, 10, 2684–2691.

[3] A. E. Khudozhitkov, P. Stange, D. Paschek, A. G. Stepanov, D. I. Kolokolova, R. Ludwig, The influence of deuterium isotope effects on structural rearrangements, ensemble equilibria, and hydrogen bonding in ionic liquids, *ChemPhysChem* **2022**, 23, e202200557.

[4] L. Hunger, L. Al-Sheakh, D. Zaitsau, S. P. Verevkin, A. Villinger, R. Ludwig, Dissecting non-Covalent interactions in carboxyl-functionalized ionic liquids exhibiting single and double hydrogen bonds between ions of like charge, *Chem. Eur. J.*, **2022**, 28, e202200949.

[5] 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.* **2022**, 13, 3556-3561.

[6] A. E. Khudozhitkov, P. Stange, A. G. Stepanov, D. I. Kolokolov, R. Ludwig, Structure, hydrogen bond dynamics and phase transition in a model ionic liquid electrolyte. *Phys. Chem. Chem. Phys.* **2022**, 24, 6064 – 6071.

[7] L. Al Sheak, T. Niemann, A. Villinger, P. Stange, D. H. Zaitsau, A. Strate, R Ludwig,.Three in one: The versatility of hydrogen bonding interaction in halide salts with hydroxyl-functionalized pyridinium cations. *ChemPhysChem* **2021**, 22, 1850-1856.

[8] 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* **2021**, 125, 17, 4476-4488.

[9] J. Neumann, R. Ludwig, D. Paschek, Hydrogen Bonds between Ions of Opposite and Like Charge in Hydroxyl-functionalised Ionic Liquids: An Exhaustive Examination of the Interplay Between Global and Local Motions and Intermolecular Hydrogen Bond Lifetimes and Kinetics, *J. Phys. Chem. B* **2021**, 125, 19, 5132–5144.

[10] M. 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* **2021**, 125, 6, 1647-1659.

[11] J. Neumann, D. Paschek, A. Strate, R. Ludwig, Kinetics of Hydrogen Bonding between Ions of Opposite and Ions of Like Charge in Hydroxy-Functionalized Ionic Liquids, *J. Phys. Chem. B* **2021**, 125, 1, 281–286.

[12] V. Overbeck, A. Appelhagen, R. Rössler, T. Niemann, R. Ludwig, Rotational correlation times, diffusion coefficients and quadrupolar peaks of the protic ionic liquid ethyl ammonium nitrate by means of ^{1}H fast-field-cycling relaxometry, *J. Mol. Liq.* ***2021***, 322, 114983.

[13] A. E. Khudozhitkov, T. Niemann, P. Stange, M. Donoshita, A. G. Stepanov, H. Kitagawa, Daniil I. Kolokolov, R. Ludwig, *Freezing the motion in hydroxy*-functionalized ionic liquids – Temperature dependent NMR deuteron quadrupole coupling constants for two types of hydrogen bonds far below the glass transition, *J. Phys. Chem. Lett.* **2020**, 11, 15, 6000–6006.

[14] H. Li, T. Niemann, R. Ludwig, R. Atkin, Effect of hydrogen bonding between ions of like charge on the boundary layer friction of hydroxyl functionalized ionic liquids, *J. Phys. Chem. Lett.*, **2020**, 11, 3905-3910.

[15] P. Honegger, V. Overbeck, A. Strate, A. Appelhagen, M. Sappl, E. Heid, C. Schröder, R. Ludwig, O. Steinhauser, Understanding the Nature of NMR Relaxation by means of Fast-Field-Cycling Relaxometry and Molecular Dynamics Simulations – The Validity of Relaxation Models, *J. Phys. Chem. Lett.* **2020**, 11, 6, 2165-2170.

[16] T. Niemann, D. H. Zaitsau,, A. Strate, P. Stange and R. Ludwig, Controlling “like-likes-like” charge attraction in hydroxy-functionalized ionic liquids by polarizability of the cations, interaction strength of the anions and varying alkyl chain length, *Phys. Chem. Chem. Phys*. **2020**, 22, 2763-2774.

[17] H. Zeng, F. Menges, M. Johnson, T. Niemann, A. Strate, R. Ludwig, Chain Length Dependence of Hydrogen Bond Linkages between Cationic Constituents in Hydroxy-Functionalized Ionic Liquids: Tracking Bulk Behavior to the Molecular Level with Cold Cluster Ion Spectroscopy. *J. Phys. Chem. Lett.* **2020**, 14, 683-688.