Angewandte International Edition Chemie

R. Ludwig

*The author presented on this page has published more than **25 articles** since 2000 in Angewandte Chemie, most recently:*
"Controlling the Subtle Energy Balance in Protic Ionic Liquids: Dispersion Forces Compete with Hydrogen Bonds": K. Fumino, V. Fossog, P. Stange, D. Paschek, R. Hempelmann, R. Ludwig, *Angew. Chem. Int. Ed.* **2015**, DOI: 10.1002/anie.201411509; *Angew. Chem.* **2015**, 10.1002/ange.201411509.

Ralf Ludwig

Date of birth:	January 16, 1961
Position:	Professor of Physical and Theoretical Chemistry, University of Rostock
E-mail:	ralf.ludwig@uni-rostock.de
Homepage:	www.ludwig.chemie.uni-rostock.de
Education:	1982–1988 studies in physics, RWTH Aachen 1988–1991 PhD with Prof. Dr. Manfred D. Zeidler, RWTH Aachen 1991–1993 Postdoctoral position with Prof. Dr. Manfred D. Zeidler, RWTH Aachen 1993–1995 Postdoctoral position with Prof. Thomas C. Farrar, University of Wisconsin–Madison 1995–1999 Habilitation with Prof. Dr. Alfons Geiger, University of Dortmund
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 behavior of organic molecules and on the structure of biomolecules. Our main goal is the prediction of macroscopic properties on the basis of molecular interactions.
Hobbies:	Soccer, drawing, FC Schalke 04

My favorite time of day is … the early morning.

I admire … people who oppose violence.

In a spare hour, I … let myself drift in my thoughts and not much else!

My favorite way to spend a holiday is … to follow my wife's suggestions.

The secret of being a successful scientist is … to appreciate the work of others.

My favorite molecule is … water in all its states.

If I had one year of paid leave I would … finish one of my promised books, and once again cheer on my favorite soccer club FC Schalke 04 live in the stadium.

The principal aspect of my personality is … to stay on the ball.

What I appreciate most about my friends is … that space and time do not matter.

My favorite painter is … Paul Cézanne.

My favorite musicians are … Steve Winwood, Eric Clapton, The Beatles, Keith Jarrett, Iiro Rantala, and Depeche Mode.

My favorite book is … *Steppenwolf*.

When I was eighteen I wanted to … get my driver's license at the first attempt.

The biggest challenge facing scientists is … making use of solar power.

My favorite drink is … water and aqueous solutions (no alcohol (which is no "solution" either)!).

If I could be anyone for a day, I would be … Paul Cézanne.

The most important future applications of my research are … based on fundamental research, which is and always will be our main task.

If I were a car I would be … a bicycle!

My first experiment was … the careless analysis of a broken mercury thermometer.

Has your approach to publishing your results changed since the start of your career?

Yes, in two respects. Today, I wait for projects to mature before publication. Only "full and rounded stories" are really useful, and will be cited accordingly. Also important is the appropriate choice of journal. What use is publication in high-impact journals that are not read by the addressed "community"? What is a suitable journal? One in which we can present and discuss the complete and well-designed research results in detail. This can also happen in the Supporting Information. The decisive factor is the transparency of the scientific results.

What do you think the future holds for your field of research?

In the future, interdisciplinary research will play an increasingly important role. In Rostock, we try to take this into account with the establishment of the first interdisciplinary faculty at a German university. The expertise in chemistry, physics, engineering, and medicine is focused on tackling interesting problems. With our expertise as physical and theoretical chemists, we contribute to the understanding of the structure, dynamics, and interactions at the molecular level whether in aqueous solutions, ionic liquids, or in catalytic processes.

My 5 top papers:

1. "Water: From Clusters to the Bulk": R. Ludwig, *Angew. Chem. Int. Ed.* **2001**, *40*, 1808; *Angew. Chem.* **2001**, *113*, 1856.
   A Review article on our old love, water! Written in the language of chemists, its content ranges from molecules to clusters, and to the unusual properties of the matrix of life. The Review needs to be updated, as surprises about water are always being discovered. At that time, I invested my entire funding from the Fonds der Chemischen Industrie into the color images of the article.
2. "Molecular Dynamics Simulations of Ionic Liquids: A Reliable Description of Structure, Thermodynamics and Dynamics": T. Köddermann, D. Paschek, R. Ludwig, *ChemPhysChem.* **2007**, *8*, 2464.
   This molecular dynamics simulation describes equally well the structure, thermodynamics, and dynamics of an ionic liquid. Up to that point, the diffusion of cations and anions was an order of magnitude too small and the ionic liquid was too rigid. The solution: parameterization of the force field against NMR reorientational correlation times of molecular vectors of the cation and of dissolved water molecules that dominantly interact with the anions. Most of the credit can be given to my former doctoral student, Thorsten Köddermann.
3. "Strong, Localized, and Directional Hydrogen Bonds Fluidize Ionic Liquids": K. Fumino, A. Wulf, R. Ludwig, *Angew. Chem. Int. Ed.* **2008**, *47*, 8731; *Angew. Chem.* **2008**, *120*, 8859.
   Peptides, proteins, or DNA are normally strengthened and tightened by hydrogen bonds (H-bonds). We demonstrated for the first time that H-bonds in ionic liquids can act as defects and thus fluidize the Coulomb system. In this way, the introduction of H-bonds into the ionic liquid reduces viscosities, melting points, and heats of vaporization, which is highly desirable for applications.
4. "Spectroscopic Evidence for an Enhanced Anion–Cation Interaction from Hydrogen Bonding in Pure Imidazolium Ionic Liquids": A. Wulf, K. Fumino, R. Ludwig, *Angew. Chem. Int. Ed.* **2010**, *49*, 449; *Angew. Chem.* **2010**, *122*, 459.
   The importance of hydrogen bonding in ionic liquids has long been controversial. With the help of far-infrared spectroscopy, we were able to study the intermolecular interaction between cations and anions and their enhancement by H-bonding. The strength and number of H-bonds was varied by a suitable choice of imidazolium cations. Supported by DFT calculations on clusters of ionic liquids, we were able to quantify the H-bonds. Although the H-bonds account for only about ten percent of the total interaction energy, they largely determine the physicochemical properties of a Coulomb-dominated fluid.
5. "Efficient Dehydrogenation of Formic Acid using an Iron Catalyst": A. Boddien, D. Mellmann, F. Gärtner, R. Jackstell, H. Junge, P. J. Dyson, G. Laurenczy, R. Ludwig, M. Beller, *Science* **2011**, *333*, 1733.
   This was our entry into catalysis research: the production, storage, and release of hydrogen as an energy source. The activities promoted by Matthias Beller at the Leibniz Institute for Catalysis are supported by us through in situ spectroscopy and DFT methods. Our tools contribute to the mechanistic understanding of the relevant catalytic processes. In this work, efficient release of hydrogen from formic acid with a highly active iron catalyst under mild conditions is reported.

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The work of R. Ludwig has been featured on the inside back cover of Angewandte Chemie:
"New Insights into the Mechanism of Photocatalytic Water Reduction by DFT-Supported In Situ-EPR/Raman Spectroscopy": D. Hollmann, F. Gärtner, R. Ludwig, E. Barsch, H. Junge, M. Blug, S. Hoch, M. Beller, A. Brückner, *Angew. Chem. Int. Ed.* **2011**, *50*, 10246; *Angew. Chem.* **2011**, *123*, 10429.