

## SOLVATION SCIENCE: A NEW RESEARCH FIELD

### A UNIFYING FRAMEWORK FOR UNDERSTANDING AND PREDICTING SOLVENT PROCESSES

The majority of chemical reactions including many important industrial processes and virtually all biological activities take place within a liquid environment. Solvents, of which water is surely the most prominent example, are able to “solvate” molecules, thereby transferring these as “solutes” into the liquid state. Solvents are not only able to provide a liquid phase for simple chemical reagents and the much more complex proteins; they have the additional ability to wet extended surfaces such as lipid membranes or metal electrodes, thereby creating interfaces.

#### Solvation research is fundamental to advance key technologies

An in-depth understanding of solvation at a fundamental level of chemistry, physics and engineering is essential to enable major advances in key technologies in order to reduce pollution, increase energy efficiency or prevent corrosion to name but a few challenges to our modern day society. In life sciences, water has been dubbed the “matrix of life” due to its role as the ubiquitous solvent, thus understanding solvation is crucial to unravelling biological function in a comprehensive way.

#### Solvents are not just bystanders

Up until now there has been a broad consensus in the literature which considered solvents to be inert media for different molecular processes. It is this concept on which most phenomenological understanding relies, such as “linear solvation free energy relations” or “continuum solvation” approaches. Transcending this traditional view, solvents are now increasingly recognized as playing an active role in their own right, ranging from solvent-mediated to solvent-controlled and even to solvent-driven processes.

The most recent advances in experiment and theory allow one to probe, describe, and even influence the structure, dynamics, and kinetics of complex solvation phenomena at the molecular level. Therefore, the time has come to develop a universal concept of solvation which can not only describe solvents in general, but is additionally able to predict properties of new solvent systems.

#### We describe and predict the solvents' role at the molecular level

The Cluster of Excellence RESOLV develops, in a bottom-to-top approach, microscopic descriptive models able to quantitatively predict the properties of solvent-mediated and solvent-driven processes. Whereas a scientific discipline traditionally develops its own models for solvation a microscopic approach guarantees direct transferability between the different scientific fields. In this new approach, solvent molecules will be considered as functional units which are employed as active species in solvent-mediated and solvent-controlled processes rather than being just inert and passive spectators.

This research encompasses investigations of the complex interplay between solutes - ranging from simple ions through peptides up to electrode surfaces - and solvents - ranging from water and supercritical carbon dioxide through to ionic liquids - at the molecular level. This requires the culmination of a broad armory of state-of-the-art spectroscopic, synthetic, engineering, and theoretical techniques, all of which are available at the RUB or have been developed and advanced further here within the last few years. The expertise present at the RUB is intensified greatly by cooperations with the [Max Planck Institute for Coal Research](#) and the [Max Planck Institute for Chemical Energy Conversion](#) in Mülheim,

the [Max Planck Institute for Iron Research](#) in Düsseldorf, and the [Fraunhofer Institute for Environmental, Safety, and Energy Technology “UMSICHT”](#) in Oberhausen.

### Linking fundamental to applied research

Any progress made in fundamental research is conveyed to applied research and ultimately to industrial processes. To enforce this important transfer of scientific knowledge two transfer centers have been launched: The [Center for Electrochemical Sciences \(CES\)](#) and the [Applied Competence Center THz \(ACC THz\)](#). This ensures the timely implementation of the knowledge gained from fundamental research into technologically relevant processes and leads to products borne out of translational cooperations with industry.

#### FURTHER INFO

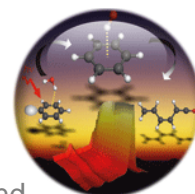
[ANGEW CHEM EDITORIAL](#)

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## RESEARCH AREA A

### UNDERSTANDING AND EXPLOITING SOLVATION IN CHEMICAL PROCESSES



The understanding of chemical reactivity is of key importance for the development and optimization of key chemical processes in both the laboratory and industry. Solvation not only changes the properties of the reactants and the products, but also affects transition states. Solvents thus influence the thermodynamics, the kinetics, and the product selectivity in liquid phase reactions. The selection of a suitable solvent frequently determines the success or failure of a chemical reaction. One example with possibly broad implications is the synthesis of enantiomeric pure products that is mandatory for any new drug development. This poses the scientific challenge of developing highly stereoselective synthetic strategies, for which the choice of a suitable solvent system is crucial. Furthermore, alternative sustainable technologies – “green chemistry” – require novel designer solvents, which reduce or eliminate the use of hazardous substances in the production and application of chemical products. A new stage in technological sorption and purification processes has been entered with the development of ionic liquids as green solvents. Nonconventional solvent mixtures are just being explored for the more effective conversion of biomass to feedstock chemicals. Focusing on strategies for the design and use of nonconventional solvents in chemical reactions will undoubtedly help to improve the efficiency in many important chemical process technologies. The new insights will have a significant impact by removing some of the crucial barriers to the development of new, sustainable technologies, including “green chemistry”.

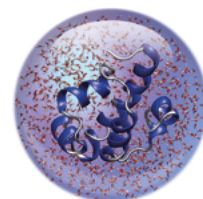
#### COORDINATOR OF RESEARCH AREA A

Please contact:

[PROF. DR. W. SANDER](#)

## RESEARCH AREA B

### CONNECTING SOLVATION DYNAMICS WITH BIOMOLECULAR FUNCTION

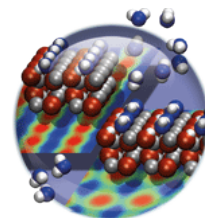


Water is the lubricant of life. Despite the fact that all life takes place in water, the treatment of water at the molecular level was not thought to be essential. Biology textbooks show proteins in front of a black background (“biology in vacuo”). However, water is not just a passive spectator solvent in biological processes, but has a vital function in most biomolecular and cellular processes. Water’s flexible network enables it to adapt its structure and dynamics. Hydration water makes significant contributions to the structure and energy of proteins and provides a responsive surrounding which allows for conformational changes. In particular, water may hold the key to the way proteins interact, fold (and misfold in ‘amyloidic’ diseases such as Parkinson’s and Alzheimer’s), bind substrates, and aggregate. Self-assembly of proteins is controlled by a delicate interplay between hydrophobic and hydrophilic interactions. Water at protein interfaces (hydration water or interfacial water) has been shown to thermodynamically stabilize the native structure of bio-macromolecules, to affect protein flexibility, and to contribute to molecular recognition in enzyme catalysis. Protein-water interactions are now known to shape the “free energy folding funnel” that drives protein folding. Connecting solvation dynamics with biomolecular function within RESOLV will open the way to achieving breakthroughs from understanding protein misfolding and formation of amyloid fibrils to rational drug design and de novo enzyme synthesis.

#### COORDINATOR OF RESEARCH AREA B

Please contact:

[PROF. DR. R. WINTER](#)



## RESEARCH AREA C

### ION SOLVATION AND CHARGE TRANSFER AT INTERFACES

Interfaces play a dominant role in molecular science. Heterogeneous catalysis is the prime example where reactions are accelerated due to the presence of surfaces including catalytically active liquid/solid interfaces. Within the last decades, surface science has triggered an impressive boost in the molecular understanding of catalytic processes. However, so far this has mainly been restricted to reactions at the gas-solid interface. Close to nothing is known about how reactants get de-solvated, intermediates stabilized, and products re-solvated along catalytic cycles at liquid-solid interfaces. It is unclear which of the concepts developed for gas-solid interfaces – if any – can be transferred to solvated interfaces. Even less understood are electrocatalytic reactions at electrified interfaces. What are the factors that quantify the rates of such universally important reactions? This seemingly simple question is far from being answered. The scientific challenge arises from the strong influence of the solvent. Improvements in chemical energy conversion depend to a large extent on the control of reactions at aqueous interfaces. One focus of RESOLV will be the investigation of the molecular basis of oxygen reduction reactions at liquid/solid interfaces. Achieving a detailed molecular understanding of these processes is of major importance, since these not only determine the performance of fuel cells, but also have an impact on corrosion, on the efficiency of metal-air batteries, and on the performance of photo-electrochemical cells.

COORDINATOR OF RESEARCH AREA C

Please contact:

[PROF. DR. D. MARX](#)