RESOLV OPENS NEW FRONTIERS IN SOLVATION SCIENCE

A UNIFYING FRAMEWORK FOR UNDERSTANDING AND PREDICTING SOLVENT PROCESSES BEYOND AMBIENT CONDITIONS, THERMAL EQUILIBRIUM, AND HOMOGENEOUS BULK PHASE.

In 2012, the Cluster of Excellence RESOLV (EXC 1069) launched Solvation Science as a new interdisciplinary field of research to provide a much-needed unifying framework for the understanding of solvation processes.

The majority of chemical reactions, including many that are central to important industrial processes, and virtually all biological processes, take place in solution. But what role does the solvent play in all these processes? RESOLV transcends the traditional view that considers solvents as being inert media in which molecular processes take place. The paradigm underlying RESOLV is to consider solvent molecules as active species, rather than just being passive spectators.

New challenges in describing and predicting the solvents' role

Seven years of research (2012-2018) have opened up new challenges in Solvation Science. We discovered that many crucial chemical transformations do not occur under ambient conditions, in thermal equilibrium or in homogeneous bulk phase.
Besides, we found necessary to lift the barriers between previously separated research thrusts (see pdf document below “RESOLV 2012-2018 - Seven years in Solvation Science”, for an overview of the previous research areas). Finally, the more we advance Solvation Science the more we find it intertwined with many other disciplines.

New goals in Solvation Science

Therefore, in 2019-2025, RESOLV (EXC 2033) tackles chemical processes far beyond homogeneous bulk phases, thermal equilibria, and ambient conditions. RESOLV takes up these emerging challenges and focuses its research on: Unravelling the mechanisms of local solvent fluctuations in heterogeneous systems (Area I), analysing how the solvent controls chemical dynamics and reactivity (Area II), and uncovering how solvation works under extreme conditions (Area III). In doing so, RESOLV bridges novel microscopic solvation concepts with macroscopic properties to boost key technological applications, such as new energy storage technologies and smart sensors. Finally, we advance the global research environment of Solvation Science and infuse this concept into other disciplines, such as astrochemistry and life sciences.

We explore new avenues of solvation, advance new technologies

In Area I, RESOLV introduces local concepts for solvation thermodynamics as well as site-specific polarity and local pH scales in nanoheterogeneous environments. The synergetic combination of experiments on local solvent properties with theoretical approaches is fundamental to the progress in this area. These concepts promise to have a strong impact on advancing molecular recognition and (bio-)electrocatalysis.

In Area II, RESOLV addresses dynamical aspects of solvation as well as ‘solvent shaping’, and proceeds to time-resolved techniques. Our goal is to tackle complex reacting systems in solution at the molecular level. This will lay the foundation for developing innovative synthesis strategies and boost the transfer of these results into bio- and process technologies.

In Area III, RESOLV considers high pressure, low temperature, and nanoconfinement as key stressors for the solvent that enable us to rigorously modulate solvation properties without changing the chemical identity of the solvent. Advancing the understanding of solvation under extreme conditions will open up new applications, ranging from organocatalysis and enzymology to increasing the shelf life of bioproducts.

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