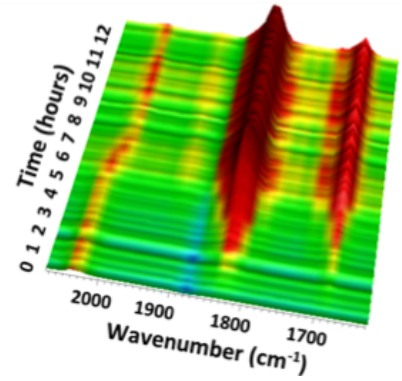
GDR « SolvATE »

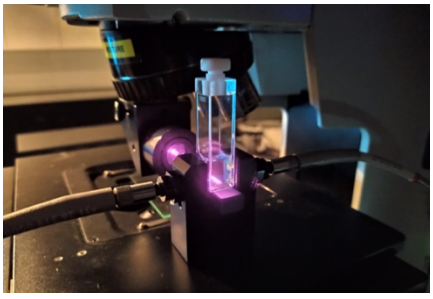
Solvation: Advances in Theory and Experiments

Goals

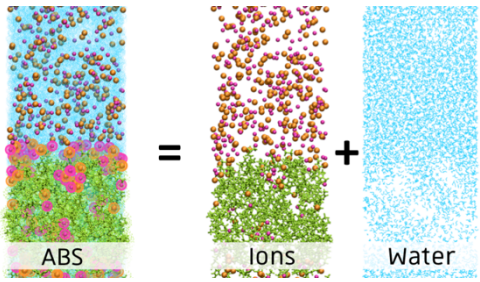
The importance of solvent effects has continuously pushed the boundaries of knowledge, in fundamental research as well as for technological applications. An essential mission of GDR SolvATE is to bring out the general problematic of solvation as a fundamental, interdisciplinary field of Chemistry and Chemical Physics. We wish to promote exchanges among French researchers, theorists and experimentalists, who study the influence of the solvent at the molecular level for the understanding of chemical processes, from complementary points of view. The organization of this dynamic community in a network of laboratories gives it an identity and leads to the emergence of cutting-edge projects involving partners outside the academic world as well.



Kinetic study (ATR-IR) of the synthesis of α-alkylidene carbonate from the catalytic coupling of CO_2 with 2-methyl-3-butyn-2-ol.



Simultaneous analysis by UV-Visible absorption and Raman scattering of an aqueous solution.



Ionic liquid-based aqueous biphasic systems: molecular dynamics simulations.

3 research themes

- Solvents in chemistry; towards a sustainable future.
- Solvation and interfaces / surfaces, nanoconfined media.
- Solvation in systems of interest in the biological and pharmaceutical field and for food processing.

100 researchers from **37** laboratories

Perspectives

The main objective of the GDR SolvATE is to promote the knowledge of the phenomena related to solvation in order to respond to well identified scientific challenges, including the optimization of industrial processes. The strength of this project lies in the interplay between theory and experience and in the implementation of interdisciplinary approaches, leading to the development of original methodologies.

The GDR scientific project revolves around three research themes.

Solvents in chemistry; towards a sustainable future.

Developing fundamental research to clarify the effect of the solvent on chemical reactivity will open important perspectives for technological and industrial applications. The interaction of specialists in the field will lead to new strategies to respond to the societal needs for environmentally friendly processes.
Coordinators: Carine Clavaguéra and Thierry Tassaing.

Solvation and interfaces / surfaces, nanoconfined media.

The chemical processes taking place at interfaces / surfaces and in nanoconfined environments reveal specificities that can be used to design a new chemistry in solution. The presence in this network of researchers is key to promote new interactions and the development of novel technologies (distillation, extraction, development of materials, electrochemistry, etc.).
Coordinators: Laurent Joly and Denis Morineau.

Solvation in systems of interest in the biological and pharmaceutical field and for food processing.

From fundamental research to process design, our researchers are working to bring innovative insights into biological phenomena that are sensitive to the environment, to enable the development of biocompatible technologies and original analytical approaches.
Coordinators: Frédéric Affouard and Anne Milet.

Highlights. Since the creation of the GDR, a priority theme has emerged and generated new dynamics, that of deep eutectic solvents, and specific actions have been mounted around this innovative subject. Another theme that has brought us new synergies is that of solvation at solid-liquid interfaces, with possible interactions with other communities (electrochemistry, energy). Finally, important theoretical developments are underway in the field of calculations of free energies of solvation and the development of efficient force fields.

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