



Einladung zum Vortrag von

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**„Solvation in ionic liquids: From chromophores
to proteins”**

The increasing demand for clean technologies resulted in a re-evaluation of many chemical processes, in particular concerning the benign and efficient usage of solvents. The application of ionic liquids can be highly beneficial in this context since organic, inorganic and polymeric materials can be dissolved by choosing the proper combination of cations and anions.

For this purpose a profound understanding of the solvent properties is mandatory and has to be gained at a fundamental level due to the overwhelming number of possible cation-anion combinations.

Polarity may be the simplest characteristic factor of solvent properties. It depends on the non-specific (e.g. dipolar) and specific (e.g. hydrogen bond) interactions between solutes and solvent molecules which can be analyzed by (polarizable) molecular dynamics simulations. In particular, the amphiphilic character of imidazolium cations can be shown.

Dielectric spectroscopy probes the macroscopic polarization of liquids applying a global electric field. The frequency-dependent dielectric spectrum reveals characteristic solvent rotations and their coupling to solute.

However, the complexity of the experimental spectra can often only be disentangled

by simulations. In solvation dynamics spectroscopy chromophores act as a local probe of the electric field. After laser excitation the chromophore changes drastically its dipole moment and the solvent response tells something about the solvation properties. Again, simulations are able to reproduce experimental data for several chromophores and solvents and draw a picture on the most important interactions.

Montag, 18. April 2016, 16:30 Uhr
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