

## **Ionic Liquids for Gas Separations and Polymer Processing**

**MARGARIDA COSTA GOMES**

CNRS RESEARCH PROFESSOR

*Institute of Chemistry at Clermont-Ferrand, BP 80026, 63171 Aubière*

*FRANCE*

*margarida.costa-gomes@univ-bpclermont.fr*

Ionic liquids are salts formed by large ions characterized by flexible and asymmetric molecular structures with a delocalization of the electrostatic charge. They constitute a vast family of liquids with large diversity of chemical structures and molecular interactions that leads to unique macroscopic properties. Ionic liquids are also structured, with persistent domains in the liquid phase: one formed by aggregates of the non-polar side chains, and the other by a network composed by charged head groups and dominated by electrostatic interactions. This segregation of polar and nonpolar domains determines the way in which solvation is understood in these media.

Simple molecular compounds, that are often gaseous at ambient conditions, have been used to assess the microscopic features (both structural and energetic) that control the dissolution process. We present several examples for which gas solubilities have provided insights on the structure and properties of different families of ionic liquids. We show how this knowledge can be used in the development of new ionic liquid media capable of selectively dissolving different molecular solutes and so act as promising separation agents.

Ionic liquids are also known to dissolve several natural polymers, in particular cellulose, under mild conditions. The interests of dissolving biopolymers are several. The first is to regenerate these compounds under different morphologies, shapes, or both. A second is to make renewable feedstocks available for subsequent chemical transformations and for the production of fuels. The third is to produce novel composites for example by blending different kinds of biopolymer. In all of these processes, a necessary step is to promote the dissolution of the biopolymers in a solvent.

We present a new approach based on the use of fundamental physical chemistry to improve the understanding of the molecular interactions between microcrystalline cellulose and an acetate-based ionic liquid, to investigate the mechanisms involved in the dissolution processes, and to perform structural and thermodynamic characterization of these systems. Experiments have been performed to determine the phase diagrams and kinetics of dissolution of the biopolymer. Both the polymeric nature of the solute and the specific physicochemical interactions between the solvent and the monomers affect the properties of the solutions. Insight into the microscopic physicochemical characteristics of the solutions – microscopic structure, preferential solvation sites – has been gained from the molecular simulation of dilute solutions of cellulose oligomers in an acetate-based ionic liquid. These are the first steps towards a more complete investigation of the dissolution and solvation processes at different scales that should contribute to design more suitable ionic liquid media to dissolve different biopolymers.