



## CYCLE DE CONFÉRENCES DE CHIMIE

Avec le concours de : *Manufacture Française des Pneumatiques Michelin*  
*Centre de Développement Préclinique, Schering-Plough*  
*Fédération de Chimie (FR2404)*  
*Section Auvergne de la Société Française de Chimie*  
*U.F.R.S.T. / Master de Chimie / Département de Chimie*

**Vendredi 14 Octobre 2011 à 14h**

*Salle C du Bâtiment de Chimie - (Site des Cézeaux)*

## Pr. JOSE NUNO CANONGIA LOPES

*Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa,  
Centro de Química Estrutural, Instituto Superior Técnico*

### Ionic Liquids from a Molecular Perspective: Liquids, Solids and Gases.

Ionic liquids are a novel class of chemical compounds generally defined as salts with melting temperatures below 100 °C and negligible vapor pressure. They also exhibit quite complex fluid phase behavior when mixed with traditional solvents. In this presentation I will try to analyze their features from a molecular thermodynamics perspective, with examples obtained experimentally<sup>1</sup> or by simulation<sup>2</sup>. The selected works bridge the liquid, gas, and solid phases spanning several years of research on themes as diverse as the vaporization, liquid-liquid demixing, solidification, and thermophysical behavior of ionic liquids, their mixtures and solutions.

The discovery that ionic liquids can be distilled at low pressure and high temperature<sup>3</sup> changed the belief that ionic liquids never occurred in the gas phase. Although their status as an important branch of green chemistry was not affected by this fact, new challenges lie on the characterization of such phase. Studies in this area corroborated the idea of ionic liquids as nano-segregated fluids, previously investigated by Molecular Dynamics (MD).<sup>4</sup>

The complex liquid-liquid and solid-liquid phase behavior of ionic liquids mixtures can be illustrated by their phase diagrams: for example, (1-ethyl-3-methylimidazolium bistriflamide + aromatic molecule) systems sometimes show the existence of extremely stable congruent-melting inclusion crystals<sup>5</sup>. Selective interactions between aromatic compounds and the cation and anion of the ionic liquid can explain such behavior. Such analyses can be extended to other systems using other experimental techniques or MD simulation.

1. L.P.N. Rebelo *et al.*, *Accounts Chem. Res.*, 2007, **40**, 1114-1121.
2. A. A. H. Padua *et al.*, *Accounts Chem. Res.*, 2007, **40**, 1087-1096.
3. M. J. Earle *et al.*, *Nature*, 2006, **439**, 831-834.
4. J. N. Canongia Lopes *et al.*, *J Phys Chem B*, 2006, **110**, 3330-3335.
5. J. Lachwa *et al.*, *Chem. Commun.*, 2006, 2445-2447.