

## Physicochemical Characterization of Fluorinated Ionic Liquids for Biomedical Applications

Fèlix Llovell <sup>C, S</sup>

*Department of Chemical Engineering and Materials Science, IQS School of Engineering, Universitat Ramon Llull,  
Barcelona, Spain  
felix.llovell@iqs.edu*

Ana B. Pereiro and Margarida L. Ferreira

*LAQV, REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa,  
Caparica, Portugal*

Rubén M. Ojeda

*Department of Chemical Engineering and Materials Science, IQS School of Engineering, Universitat Ramon Llull,  
Barcelona, Spain*

João M. M. Araújo and Luis P. N. Rebelo

*LAQV, REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa,  
Caparica, Portugal*

Manuel M. Piñeiro

*Departamento de Física Aplicada, Faculdade de Ciencias, Universidade de Vigo, Vigo, Spain*

Lourdes F. Vega

*Gas Research Center and Chemical Engineering Department, The Petroleum Institute, Khalifa University of Science  
and Technology, Abu Dhabi, United Arab Emirates*

The interest in fluorinated ionic liquids (FILs) in the biomedical field has arisen in areas where perfluorocarbons (PFCs) find relevant applications. PFCs are used as *in vivo* gas carriers, and in liquid ventilation or artificial blood substitutes formulations. [1] This work focuses on the design and development of FILs to replace fully or partially the PFCs present in the emulsions used as oxygen therapeutics. A combined theoretical-experimental approach has been used to characterize these compounds considering their thermodynamic behavior in the presence of water and respiratory gases. The phase equilibria of different imidazolium and pyridinium cations combined with the  $[\text{C}_4\text{F}_9\text{SO}_3]^-$  and  $[\text{C}_4\text{F}_9\text{CO}_2]^-$  anions with water has been studied to evaluate the feasibility of partially replacing PFCs-in-water emulsions, which are currently used as oxygen carriers. Additionally, the critical aggregation concentrations for these FILs in water have been determined using ionic conductivity, surface tension, and isothermal titration calorimetry. [2] Additionally, the self-assembled structures of FILs in water have been evaluated using transmission electron microscopy. [2] Part of this experimental information has been modelled using the soft-SAFT equation of state (EoS). A molecular model based on the analysis of the distribution charges on the anion has been proposed and optimized to find a reliable set of parameters to describe the FILs family, revealing good agreement with experimental data and a high degree of transferability. [3] The model has been later tested to describe the liquid-liquid equilibrium of water + FILs mixtures. A theoretical evaluation of the interfacial tension and the viscosity of these compounds is also provided. Finally, this molecular model has been used to predict the solubility of the respiratory gases in these FILs. This characterization allows the search for a FIL that might be the best candidate to use as an artificial gas carrier.

### References:

[1] Riess, J. G. Chem. Rev. 2001, 101, 2797-2919; [2] Pereiro et al. Langmuir 2015, 31, 1283-1295; [3] Pereiro et al. Chem. Phys. Chem 2017, 18, 2012-2023.

Acknowledgements: The financial support from FCT/MCTES (Portugal), through Investigador FCT 2014 (A.B.P. and J.M.M.A.), and projects PTDC/QEQ-EPR/5841/2014, PTDC/QEQ-FTT/3289/2014, IF/00210/2014/CP1244/CT0003, UID/QUI/50006/2013.