Molecular Thermodynamics Lab

Supervisor(s): Luís P. Rebelo and Ana B. Pereiro (luis.rebelo@itqb.unl.pt and anab@itqb.unl.pt)

TITLE: Highly Fluorinated Ionic Liquids in the development of Biomaterials

BACKGROUND

The development of biomaterials to treat, repair or reconstruct the human body is an increasing important component of materials research. Collaboration between materials researchers and their industrial and clinical partners is essential for the development of this complex field.

Research in this area was driven by the potential applications of such materials in medicine and biology. Fluorocarbon compounds have been developed as media for liquid ventilation, drug delivery systems, injectable oxygen carriers and contrast agents for ultrasound imaging. From a more fundamental standpoint, these materials are being investigated for assessing and understanding the impact that fluorinated components have on the formation, stability, structure and properties of colloidal systems in comparison with their hydrocarbon counterparts.

A large variety of colloidal systems involves highly fluorinated components comprising a range of self-assemblies (vesicles, tubules, helices, ribbons, etc..) and diverse types of emulsions (direct, reverse or multiple emulsions, microemulsions, gel emulsions, waterless emulsions, etc..) made from fluorinated amplhiphiles.

OBJECTIVES

The aim of this project is to evaluate the possible application of fluorinated ionic liquids as biomaterials for biomedical purposes.

With this goal in mind, thermodynamic and thermophysical properties will be measured for pure fluorinated ionic liquids and their mixture. Thermal properties, viscosity and density of these compounds will be analyzed in Task 1; refractive index, surface tension and ionic conductivity in Task 2; partition coefficient in Task 3; solubility in Task 4; and diffusion coefficients in Task 5.

On the other hand, the critical micelle concentration for different fluorinated ionic liquids which present cations and / or anions with tensioactive properties will be also determined in Task 6.

PROJECT DESCRIPTION

Ionic liquids have become a green media for engineering applications due to exceptional physicochemical properties, such as their practically nonvolatile nature, null flammability, low melting point, high ionic conductivity, and thermal and electrochemical stability. Although the number of publications on ionic liquids has witnessed exponential growth, their chemical diversity has not been exhaustively explored, namely the fluorinated ionic liquids field. The use of fluorinated ionic liquids is of particular interest in areas where fluorocarbon compounds find relevant applications such as imaging agents, fluorocarbon gels, nanocompartmented supramolecular architectures and colloids, control and stabilization of emulsions, microbubbles and other colloids, pulmonary delivery of drug and genes and oxygen therapeutics, where these compounds are used as gas carriers in liquid ventilation and intravenous formulations.

The specific physicochemical properties of perfluorocompounds have triggered numerous applications in the field of biomedical. Some of these properties influence the amount and diffusivity of gases (solubility, diffusion coefficients), others influence how the liquid moves within the lung (vapor pressure, surface tension, density and viscosity) and others influence the biodistribution of these compounds (partition coefficient, lipid solubility).

Following these trends, it is of great importance to develop neoteric ionic liquids with fluorinated alkyl chains that can boost their application into this important research area. Two main objectives will be pursued in this project: on the one hand these new fluorinated ionic liquids will be able to replace, partially or totally, the perfluorocompounds used for biomedical purposes; on the other hand, long chain fluorinated ionic liquids will be used to promote the stability of various colloidal systems, including different types of emulsions, vesicles and tubules that also show promise for controlled release drug delivery due to the strong tendency of these molecules to self-assemble. The expected nanostructuring effect, promoting fluorinated domains, will be addressed in the first case, while in this last application the fluorinated domains of the perfluorocompound-in-water emulsions are expected to promote a higher capacity to solubilize gases, as oxygen, than when other surfactants are used.

The potential of fluorinated ionic liquids is large and unexplored, and thus can unleash a complete turnaround in the field of biomedical applications.

<u>TIMELINE</u> (use fill tool for the cells)

	Month 1	Month 2	Month 3	Month 4	Month 5	Month 6	Month 7	Month 8	Month 9	Month 10
Task 1	■	■	■							
Task 2		■	■	■						
Task 3			■	■	■					
Task 4				■	■	■				
Task 5					■	■	■			
Task 6						■	■	■		
Thesis								■	■	■