

Soft.Matter@PT 2015

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Expertise: Interfaces and wetting of simple fluids and liquid crystals

	Colloids	Liquid Crystals	Polymers and Gels	Interfaces, surfactants	Foams, emulsions	Granular materials	Biological	Lipid Bilayers
Experimental								
Computacional							✓	✓
Theoretical							✓	✓

Description of expertise:

- Theoretical/Computational Chemistry and Biochemistry
- Molecular Mechanics; Quantum Mechanics; Force Field Development; Molecular Dynamics; Continuum Electrostatics; Molecular Docking; Membrane Biophysics.
- The influence of pH and reduction potential in biomolecules; The protonation/conformation coupling in lipids and its influence in the structure of biological membranes

Selected Publications (max 5):

- *Constant-pH MD of an oleic acid bilayer*, [J.Chem.Theory Comput., 11, 2367 \(2015\)](#).
- *Ionic strength in charged lipid bilayers*, [J.Chem.Theory Comput., 10, 5483 \(2014\)](#).
- *Protonation of DMPC in a bilayer*, [J. Chem. Theory Comput., 10, 2176 \(2014\)](#).
- *Conformational behavior of peptide dendrimers* [J.Am Chem.Soc., 133, 5042 \(2011\)](#).
- *Constant-pH/redox MD in Cyt.c₃*, [J. Am. Chem. Soc., 131, 12586 \(2009\)](#).