Research Project no. MSMC1 (Area: Molecular Systems and Materials Chemistry)

Minimum duration of the research internship: 3 months

Molecular Modelling and Simulation of novel Ionic Liquids

Prof. José Nuno Canongia Lopes

E-mail: jnlopes@tecnico.ulisboa.pt

Molecular modelling and simulation include computational techniques developed within the frameworks of quantum or statistical mechanics that are able to analyse the links between the macroscopic properties of matter and its characteristics at a molecular level. Modelling and simulation studies are traditionally used either as predictive or interpretative research instruments but in the case of ionic liquids (ILs)—a relatively recent research front—they have also assumed the role of exploratory tools leading to some discoveries that were only later corroborated by experimental evidence. For instance, one of the first works dealing with the recognition of ILs as nano-segregated fluids originated from molecular dynamics (MD) studies [1], reported in the sequence of the development of a systematic force field for ionic liquids [2,3]. In other words, the knowledge about the physical chemistry of ionic liquids is rapidly advancing through the interplay between experiments, theory, and modelling, each providing challenges, guidelines, and checks to the others.

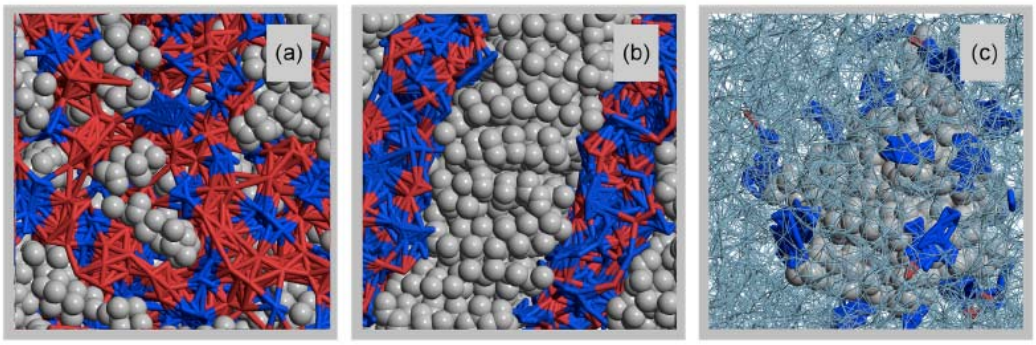

Fig.1 Simulation snapshots depicting different examples of structures present in ILs: (a) bulk IL; liquid crystalline IL; (c) IL micelle in aqueous solution. All images have been represented in the same scale, the side of each square measuring 3.5 nm. The polar moieties of the IL are represented as blue and red coarse mesh (cations and anions, respectively), the non-polar alkyl side chains of the cations as light grey space-filled atoms, water molecules as a fine mesh.

In this project the student will be working in the day-to-day tasks that are at the core of the research activity of the molecular modelling and simulation group led by the supervisor of this project. These include force-field parameterisation and validation, the set-up and testing of MD runs, and the collection and interpretation (data farming) of simulation trajectories. The object of study will be a selected ionic liquid system that will be at the forefront of research interests of the group at the time of the project. These can comprise for instance the study of novel mixtures of ionic liquids with molecular solvents, the structure of ionic liquids that form liquid crystalline phases, or the properties of ionic liquids under confinement (films, monolayers, at interfaces).

References

1. J. N. Canongia Lopes, A. A. H. Pádua (2006) *J. Phys. Chem. B* **2006**, *110*, 3330.
2. J. N. Canongia Lopes, J. Deschamps, A. A. H. Pádua (2004) *J. Phys. Chem. B* **2004**, *108*, 2038.
3. J. N. Canongia Lopes, A. A. H. Pádua (2006) *Theor. Chem. Acc.* **2012**, *131*, 1129.