Ionic Liquids – A Piece in the Puzzle of Developing Energy Sources

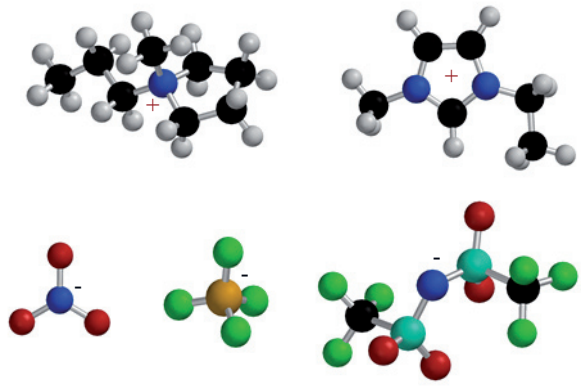
By Dr. Bodil Ahlström

One of the major challenges the modern society is facing is to meet the rapidly increasing energy demand in an environmentally sustainable way. It is essential to invest in renewable technology for electricity generation, storage and transport.

Rechargeable lithium-ion batteries, with their high energy density, high power and their good ability to be recharged many times, take up a large part of the global market share of rechargeable batteries, much because of their widespread use in mobile phones and laptops etc. Their market share is expected to increase even further as they are promising components in electric grids and electric vehicles.

Currently, commercial lithium batteries use organic solvent based electrolytes. These electrolytes allow the realization of high performance batteries. However, since the solvents are flammable, their use poses serious safety risks and strongly reduces the batteries operational temperature range. As a result, there has been much interest in recent years to replace organic solvents with ionic liquids (ILs).

Ionic liquids represent an interesting class of liquid material that consists entirely of ions and by definition melts below 100 °C. During the last decade, ILs have been in focus for an increasing interest as electrolytes in electrochemical devices such as lithium batteries, fuel cells, solar cells etc. where they have the potential to contribute to the development of more potent, safer and environmentally benign materials. ILs generally exhibit high ionic conductivity, high thermal and chemical stability, a wide electrochemical window, and low toxicity.



An IL typically consists of a bulky organic cation and an inorganic anion. Examples of common types of ions are shown. Upper left to right: cations based on pyrrolidinium and imidazolium. Lower left to right: the anions nitrate, tetrafluoroborate and bis(trifluoromethanesulfonyl)imide.

Given the large number of cations and anions available today, the dual combination leads to a huge number of possible ILs, most of them not yet synthesized. Therefore, it is highly desirable to use computational techniques and modelling for predicting physical properties for any given ion combination. Such properties, e.g. liquid temperature range, vapor pressure and density can be investigated by for instance Monte Carlo simulation and Molecular Dynamics simulation methods. This allows for a rational design of new IL-based materials and a reduction of the need of time consuming trial and error syntheses of ILs.

One of the key factors for an IL to be suitable for electrochemical applications is high conductivity. Conductivities and other dynamic properties (e.g. viscosity, diffusion) can be calculated by Molecular Dynamics methods.