Project title: Understanding self-aggregation on long length scales in ionic liquids using computer simulations
Supervisor name(s): Dr Martin Bates, Dr John Slattery and Prof Duncan Bruce
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Introduction: Ionic liquids (ILs) are molten salts with melting temperatures below 100 °C, although most that are currently of interest are liquid at room temperature or below. They have received a great deal of interest over the last ten years or so because of their interesting, and sometimes unique, combination of physical properties and because of their wide range of potential applications: from their use as potentially green solvent systems to electrolytes in batteries and solar cells and in biomass processing. New ILs are now being designed to have liquid-crystalline phase (LCILs), in which the molecules self-organise with long-range order. Depending on the phase structure these have a range of possible applications as electrolytes, solvents and in gas separation/storage.

Project: The student will investigate molecular self-aggregation and its effects on the long range structure of liquid-crystalline ionic liquid systems. The student will do this both experimentally and computationally, with the common goal of understanding the structure of LCILs. Computationally, the student will build on existing atomistic models to develop new coarse grained models for simulating LCILs. A major drawback of atomistic models is that they cannot reach the large length or timescales necessary for investigating the structure of LCILs. By developing simplified, but robust, coarse grained models, the student will be able to probe the formation of the ordered phases of LCILs. Experimental data will primarily be drawn from X-ray and neutron scattering experiments using existing and novel materials from the JMS and DWB groups; SWAXS (York) and SANS at ISIS (Oxford) and ILL (Grenoble). The student will therefore be in a position to collect and analyse their own experimental data and use computational techniques to probe and predict the molecular self-aggregation responsible for the long range structure of the liquids and, hence, the phase behaviour.

Training: No background in computational chemistry is necessary. However, as the project has a computational aspect, the student should have an interest using computers for both simulation and experimental analysis. Full training will be given on practical high-performance scientific computing (linux, chemistry software, programming, parallelisation, etc) as well as on running and analysis of X-ray and neutron scattering experiments. Our full range of graduate Chemistry Courses, as well as courses on scientific writing, presentation skills etc. are also available for further training. The student will be expected to network at Chemistry events and present their work as a poster or oral presentation. These will range from group meetings and one day symposia, to annual poster sessions organised by the Department of Chemistry, to termly seminars organised by the postgraduate community. The student will also be encouraged to attend both conferences on ionic liquids and more general major international conferences during their PhD, such as COIL and EuCheMS.

Application closing date: 17:00 on 11 January 2017
Interview date: 15 February 2017

Funding source: EPSRC or Department of Chemistry
Funding scheme (if any): DTG/Teaching Studentship
Funding Types: Competition
Eligibility: UK

All research students follow our innovative Doctoral Training in Chemistry (iDTC): cohort-based training to support the development of scientific, transferable and employability skills
For more information contact chemgrad@york.ac.uk or see our web page: http://www.york.ac.uk/chemistry/postgraduate/
The Department of Chemistry holds an Athena SWAN Gold Award and is committed to supporting equality and diversity for all staff and students.