Application for a TSM-DTC funded PhD studentship

Please complete this form electronically
and submit to Lilian Wanjohi (l.wanjohi@imperial.ac.uk)
by Friday January 8, 2010

1st supervisor
Name: Patricia Hunt
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Name: Tom Welton
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3rd supervisor
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Please complete the following:

1. Project title: New methods and novel materials: Ionic Liquids

2. Project abstract (≤ 200 words please and please add 1 or 2 key references)

The focus of this project is a multiscale investigation of ionic liquids.

Room temperature ionic liquids are novel solvent and electrolyte materials being explored for use in a wide range of applications from electronic devices to industrial chemistry. Examples of potential applications are very diverse; dissolving wood in pulp and paper processes, acting as electrolytes in solar cells, preserving proteins, electro deposition of "insoluble" metals, and saving energy by replacing cryolite in aluminum production. Key to all of these applications is the extraordinary ability of the ionic liquid to dissolve or solvate another entity (the solute). However, the solvation characteristics of ionic liquids are not at all well understood. The focus of this project is to investigate solvation in ionic liquids: What is it that makes ionic liquids such impressive solvents and electrolytes?

In this project we will use quantum chemical and molecular dynamics methods in concert with experimental data to develop an understanding of the physics and chemistry of

solvation in ionic liquids. Prof Welton and Dr Hunt have a strong record of highly successful collaborative projects using simulation and experiment cooperatively. Experimental data will be provided to verify computational results, while molecular level insights from the calculations will be used to develop robust explanations for observed phenomena that are currently not understood.

Understanding the process of solvation in ionic liquids will enable the prediction and control of ionic liquid properties, and potentially the identification of new materials and applications involving ionic liquids. An active association with BASF will allow any breakthrough to be rapidly implemented in an industrial environment.

P. A. Hunt and T. Welton, Chem. Eur. J. **12**, 6762 (2006)
P. A. Hunt, J. Phys. Chem. B **111**, 4844 (2007)

3. What is the multi-scale nature of the project? (≤ 100 words please)

This projects spans from the quantum to the observable, we start from a molecular description and move through macroscopic to experimental phenomena. We start by developing a firm understanding of the electronic structure at a fundamental molecular level (quantum chemical), we then develop effective potentials for use in molecular dynamics simulation (classical MD) which will allow us access to larger systems and dynamic behavior and we will complete the processes by comparison with experimental phenomena. This is unlikely to be a linear process but one in which the results from one aspect inform on and change aspects in the other areas "on the fly". A key and unique part of this project is the cooperative theoretical and experimental approach, the systems simulated will be in part determined by which experiments can actually be carried out, the experimental studies undertaken, will be determined (in part) by the systems that can be reasonably simulated.

4. How do the expertises of the supervisors complement each other? (≤ 100 words please)
Supervisors have a specialization at different levels of the multi-scale approach.

Hunt: Quantum mechanics (electronic structure theory: density functional and higher levels) Classical atomistic and ab-initio molecular dynamics simulations of liquids.
Welton: Experimental studies of ionic liquids
Both: An emphasis on developing models of understanding employing concurrently both computation/simulation and experiment (for example we hold joint group meetings)
Dr. Schäfer: Industrial collaborator, during the course of their studies the student can expect to visit BASF and to be welcomed into the Scientific Computing / Quantum Chemistry group of Dr. Schäfer.

5. Is there a self-contained 12-week MSc project that would usefully initiate this PhD project? (If the answer is no the project will not be offered as an MSc project)

Yes! The student will be given a "taster" from each stage of the project, applying the relevant techniques to a simple model system and comparing their results to those in the established literature. Perform quantum chemical calculations on an ionic-liquid ion pair with a dye molecule (in ground and first excited states). Experimental information obtained

from the dye's uv-vis spectrum provides information on the nature of the solvent (H-bonding ability, polarizability etc). Investigate the electronic structure using a range of techniques and relate this to relevant literature. (4 weeks) Then generate an effective semi-empirical intermolecular potential (point charge model) for the ionic liquid ion pair with dye in an excited and ground state. (2 weeks) Use classical MD to explore the liquid dye interactions and dynamics. (4 weeks) Compare to experimental data and develop a description for the dye-ion interactions. (2 weeks) (The experimental analysis of the dye response in the solvent is straight forward, and the student could spend a week shadowing a more experienced student in the lab as they do the experiment). The literature evaluation will give the student an appreciation of the current state-of-the-art in this field. The full project implements this process for a larger range of species involving more complex interactions (for example other solutes (such as metal ions) and binary ionic liquid mixtures).