

**"Molecular solvents over heterogeneous surfaces and ionic liquids
in the bulk - experimental and theoretical study of hydrogen
bonding systems"**

Dr. T. Youngs
(t.youngs@qub.ac.uk)

Atomistic Simulation Centre
Old Physics Building
Queen's University Belfast
Belfast, BT7 1NN, N.I.
U.K.

Ionic liquids represent an interesting class of solvents for structural studies to focus upon, even if their potential practical uses are occasionally over-hyped. The presence of hydrogen bonding in the liquid state is now well accepted and, in the context of experimental structural studies, adds another subtlety by which to challenge any data refinement procedures. An overview of hydrogen bonding in ionic liquids is provided, the resulting effects on the liquid state are discussed, and recent neutron diffraction data and its refinement on specific ionic liquid systems is presented and discussed.

On an entirely different note, the underlying oxide supports used in heterogeneous catalysis are often considered the prevalent influence on the structure of hydrogen bonding molecular solvents. Simulation studies of partially hydroxylated surfaces have shown, however, that surface heterogeneities can have a significant effect on the structure also. Molecular dynamics simulations of thin films over model ionic surfaces containing 'catalyst' patches will be presented, extending the idea of liquid structuring arising from such inhomogeneities on the surface.