



~~Special Polymer Physics Seminar ~~

Dr. Patricia Hunt

Department of Chemistry,
Imperial College, London, U.K.

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301 Steidle Bldg.

Understanding Ionic Liquids: From the Electronic Structure Up

Room temperature ionic liquids are promising new solvents and electrolytes with a number of appealing physical and chemical properties. These include; low vapor pressure, large liquid range, thermal and electrochemical stability and a wide electrochemical window. Ionic liquids are therefore of particular interest as advanced functional materials and engineering fluids (additives, storage media, fuels and lubricants) and as electrolytes in electrochemical applications (Li-batteries (for cell-phones), fuel-cells (for the hydrogen economy) and photo-voltaic cells (solar energy)). Of more interest to synthetic chemists are highly favorable solvating properties, tuneable miscibility, and an ability to selectively direct reactivity.

A key feature and advantage of ionic liquids is the potential ability to tailor physico-chemical properties by varying the constituent ions. However, advances are being hampered by an inability to predict, or even rationalize, ionic liquid properties. Computational studies can help by establishing a link between the properties of constituent ions and the resultant ionic liquids. In this talk I will focus on the useful information that can be obtained from quantum chemical studies. I will show how we have used this knowledge to rationalize the "unexpected" properties of a newly synthesized IL, and I will show how we have been able to resolve a key experimental discrepancy raised when my collaborators obtained apparently contradictory experimental results from two complementary techniques applied to the *same* ionic liquids.