



Einladung zu einem Seminar über Neutronenstreuung

(ETH-Veranstaltung Nr. 402-0540-002 im Wintersemester 2007)

Date: Tuesday, March 4, 2008, 10:30

Location: Paul Scherrer Institut, Area West, Bldg. WHGA/121

Speaker: Prof. Dr. Barbara Kirchner Wilhelm-Ostwald Institut
für Physikalische und Theoretische Chemie Universität Leipzig

Title: **“Dynamics and intermolecular forces in ionic liquids from
theoretical considerations“**

Abstract:

Ionic liquids (IL) are a paradox, i.e. they are salts (supposed to be solid) in a liquid like state. They interact typically for both forms (ionic like a solid as well as associated like a hydrogen bonded liquid) and belong to neither. We try to understand how ionic liquids emerge by comparing them gradually to a salt (NaCl) that is solid at room temperature, respectively by comparing them to molecular liquids or to hydrogen bonded systems.

The most simple picture of ILs concentrates on the fact that they are charged species. However, we can show that other important forces are present in ionic liquids. Static quantum chemical methods might describe the electronic structure well, but they are not suited to describe the liquid phase. Molecular dynamics (MD) simulations can describe the liquid phase, but either neglects cooperative (traditional MD) or dispersion effects (first-principle MD).

Another problem is associated with the property that ionic liquids are viscous which enforce large simulation times. This presentation shows characteristics of ionic liquids and the problems which can occur when investigated with different methods.

Contact: Jan Peter Embs WHGA/112, Tel. 056 310 53 92; e-mail: jan.embs@psi.ch