Priority Programme

“Material Synthesis near Room Temperature”

Project Description – Project Proposal

Ionic Liquids in the Synthesis and Tuning of Porous Materials: Knowledge-based Design of Properties Using a Combined Experimental and Theoretical Approach

Participant	**Prof. Dr. Barbara Kirchner**
Institution	Rheinische Friedrich-Wilhelms-Universität Bonn Institut für Physikalische und Theoretische Chemie Mulliken Center for Theoretical Chemistry Beringstraße 4 53115 Bonn Telephone +49 228 73-60442 Fax +49 228 73-9064 E-Mail kirchner@thch.uni-bonn.de
Participant	**Prof. Dr. Annegret Stark**
Institution	Technische Universität Darmstadt Eduard-Zintl-Institut Fachgebiet Physikalische Chemie Alarich-Weiss-Straße 8 64287 Darmstadt

Summary of proposal

This project is a bilateral project between PD Dr. Annegret Stark (Leibniz-Institute of Surface Modification, Leipzig) and Prof. Dr. Barbara Kirchner (Universität Bonn). The expertise of experimentalists and theoreticians is hence combined. Research focus 1 (RF 1) of this project is concerned with the investigation of ionic liquids (ILs) as solvents and structure-directing agents in the synthesis of zeolites. It is the goal to understand the prevailing and governing interactions on molecular level, contributing to an understanding of the solvation and crystallisation mechanism leading to high selectivities in the resulting framework geometry. RF 2 investigates the properties of ILs in confinement, i.e. in porous materials. The aim is to provide a detailed knowledge of the interfacial structure and interactions between porous inorganic materials and ILs, leading to deviations from bulk liquid properties (density, melting point etc.). Investigations will be carried out systematically, including series of homologues of ILs where the cation, the anion or the cation substituent are successively altered. In RF 1, we will extend our prior studies from AlPOs to SAPOs, MAPOs and finally to true zeolites (aluminosilicates), to shed light into the limits of ionothermal zeolite synthesis regarding precursors, ionic liquid types and resulting framework types.In RF 2, we will investigate the properties and orientation of the IL in confinement in dependence of the ionic liquid structure (homologues series), the nature of the support (pore size, geometry, chemical composition) and the ionic liquid loading. Furthermore, the pore filling mechanism with respect to the type of support will be studied. The following research questions are in the centre of the project:

1. Which structural features of the IL (type of cation, cation substituent, type of anion) affect the resulting framework type? Which interaction types prevail?
2. Can the IL be designed to generate new framework structures?
3. What is the role of the mineralizer and can it be substituted by an IL function?
4. Can the (low pressure) ionothermal synthesis be converted in a continuous synthesis protocol?
5. What is the effect of the confinement on the physicochemical properties of the IL?
6. How does the confinement affect the orientation of the IL?
7. How does the IL constitution (i.e. its anion, cation, cation substituent) affect the orientation in confinement, compared to the bulk liquid?
8. Is the pore filling mechanism dependent on the IL?