

## Workshop

### **“Application of X-ray Absorption Spectroscopy in (Solid-state) Chemistry – XAS Data Reduction and Analysis”**

After a short introduction into the basics of X-ray absorption spectroscopy (XAS) (physics, experimental, and data reduction) the workshop will focus on the practical aspects of XAS data analysis (one-third theory, two-thirds hands-on). We will work together on selected examples illustrating the fundamental data reduction steps (e.g. calibration, background removal,  $\mu(0)$  fit, FT) and data analysis steps (XANES reference fitting, principal component analysis, EXAFS refinements using experimental and theoretical phases and amplitudes). The workshop is intended for beginners and XAS user with a basic knowledge about X-ray absorption spectroscopy and XAS data analysis.

#### „Programme“

#### **Thursday, Sept. 8, 2005**

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| 9:00  | Introduction to XAS, Experimental, XAFS Data reduction and analysis  |
| 10:30 | Health Break   |
| 10:45 | „Hands-on“ Selected examples for data reduction and analysis<br>(EXAFS: calibration, background, $\mu(0)$ fit,<br>XANES: reference fitting, PCA, profile fitting;)   |
| 12:30 | Lunch  |
| 13:30 | “Hands-on”: EXAFS and XANES-Analyses<br>(XAFS fits with theoretical phases and amplitudes, single and multiple scattering, PCA of “real” samples, evaluation of multiple scattering paths in crystalline and disordered solids, XAFS analysis of phase mixtures) |
| 15:15 | Health Break   |
| 15:30 | Continue “hands-on” XAS data reduction and analysis  |
| 17:00 | Closing  |