PAUL SCHERRER INSTITUT

Invitation
to an ENE-Seminar

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Place: OSGA/EG 6

New Insights in Homogeneously Catalysed Selective Polymerisation Reactions using Novel X-ray Spectroscopy Methodologies

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X-ray Absorption spectroscopy (XAS) is a technique for detailed structural and electronic characterisation of materials. Its strengths include the ability to perform experiments in situ/operando (variable temperature and pressure) and time-resolved. The technique is element specific and it does not require long-range order so amorphous systems and solutions can be studied, which makes it a powerful techniques in catalysis. New technique developments are centered on increased energy resolution and thereby increased information content as well as increased time-resolution. The techniques are developed as tools in homogeneous catalysis, where the use of XAS is still limited.

So far, XAS has been mainly used to obtain a structural picture whereas the electronic structure is often poorly understood. Moreover, the major disadvantage of XAS is that it determines an average of all the different structures present, as such complicating the analysis and interpretation. New developments in XAS using new instrumentation and data acquisition methods while selecting specific x-ray energies provide more detailed electronic information as has been feasible so far. The charges on and bonding between atoms can now be visualised and their distribution and orientation studied, creating ultimately a 3-dimensional electronic picture or movie of the material.

Fast moving monochromators and energy dispersive acquisition methodologies have enabled the study of catalytic systems down to the millisecond time scales and reaction mechanisms have been obtained. For example, time-resolved XAFS in combination with UV-Vis has allowed detailed characterization of homogenous reaction intermediates in situ and time-resolved, making it a powerful tool in revealing reaction mechanisms.

These novel XAS techniques, both theory and in situ/operando instrumentation, are currently being developed and applied to catalytic systems. The properties and catalytic performance of homogeneous catalysts are studied during their catalytic activity, with a combination of complementary (spectroscopic) techniques. The influences of different ligands on the structural and electronic properties of the active site are investigated. Detailed insights in reaction mechanisms are obtained. Here, new insights in selective polymerisation reactions using Cr and related catalysts are presented.