

# Réunions scientifiques

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Séminaire SOLEIL

# Shining synchrotron light on catalysts at work

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Invité par Valérie BRIOIS

## Vendredi 5 avril à 14h00 Grand Amphi SOLEIL

Catalytic processes play an important role in the chemical industry because more than 90% of all chemical products undergo at least one process step which involves catalysis. With the present shift and demand for new energy resources, the steadily increasing population and the demand for cleaner and greener processes, a number of challenges have to be met where catalysis plays a key role. During the catalyst development the vision is to move from trial-and-error methods more towards an understanding of the catalytically active species and its design. In fact, the development of new characterization methods and novel approaches has often pushed the development in catalysis in the past.

Synchrotron light has a long tradition in the characterization of materials. In particular, structure-performance relationships gained by studying catalysts at work are considered the key to further development of catalysts. Here, the role of *in situ* and *operando* spectroscopy will be highlighted using examples from X-ray absorption spectroscopy and gas phase reactions to demonstrate the challenges and the opportunities of this approach. Considering that many fine chemical reactions are conducted in liquid phase and a number of industrial reactions are performed at higher pressure, the extension of this idea to those reaction conditions is important as well and is discussed in the next step. In certain cases a variation of the catalyst structure can occur inside a catalytic reactor as a result of temperature or concentration gradients. In addition, rapid structural changes can occur during activation, ignition and reaction. This additionally requires spatially and time resolved structural information of the catalyst materials. A prominent example is the partial oxidation of methane over noble metal based catalysts, interesting for the production of hydrogen from natural gas. In order to obtain spectroscopic information on the oxidation state in a spatially resolved manner inside the catalytic reactor scanning and full field X-ray microscopy with spectroscopic information based on X-ray absorption spectra were used. In addition, the temperature profile was analysed using an IR-camera and the catalytic performance using mass spectrometric analysis. In a more recent experiment the ignition process of the partial oxidation of methane was followed both by time-resolved QEXAFS studies and detection of the change in X-ray absorption giving information in the structural changes in a 2-dimensional way.

#### References

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[3] J.-D. Grunwaldt, J.B. Wagner, R.E. Dunin-Borkowski, "Imaging catalysts at work: A hierarchical approach from the macro- to the meso- and nano-scale", ChemCatChem, 5: 62–80 (2013) [4] J. Stötzel, R. Frahm, B. Kimmerle, M. Nachtegaal, J.-D. Grunwaldt, "Oscillatory Behavior during the Catalytic Partial Oxidation of Methane: Following Dynamic Structural changes of Palladium using the QEXAFS Technique", J. Phys. Chem. C, 599, 599 (2012).

[5] D. Klukowski, P. Balle, B. Geiger, S. Wagloehner, S. Kureti, B. Kimmerle, A. Baiker, J.-D. Grunwaldt, "On the mechanism of the SCR reaction on Fe/HBEA zeolite", Appl. Catal. B 93, 166 (2009).



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