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Analysing Big Data: QXAS on Pt-Ga catalysts

Aim

As measurements become more complex and acquisition times get reduced, BIG data are increasingly encountered in research. This is for instance the case for Quick X-ray Absorption Spectroscopy measurements, where full spectra are recorded in less than seconds, quasi-simultaneously for several elements. In order to master these large amounts of data, new analyses methods are required, allowing for swift data visualisation, automated data treatment and accessible interpretation.

Justification

Promoted Pt catalysts are very effective to catalyze propane dehydrogenation, a major route to selectively produce propene. By adding a small amount of CO_2 to the feed as soft oxidant, carbon formation can be reduced and the equilibrium shifted to enhance selective production.
Ni-Fe catalysts are known to rearrange under oxidizing or reducing conditions. Pt-based catalysts are expected to behave similarly, but so far, their behavior under oxidizing conditions has hardly been examined. In order to identify their restructuring and the Ga role, multiple Pt-Ga catalysts have been examined using Quick-X-ray absorption spectroscopy (QXAS) at both the Pt-L_{III} and Ga-K edge. XAS allows to examine the local environment around Pt and Ga in these bimetallic catalysts, even during treatment or reaction (reduction, oxidation, reverse water gas shift, redox cycling), see Figure 1 & 2.

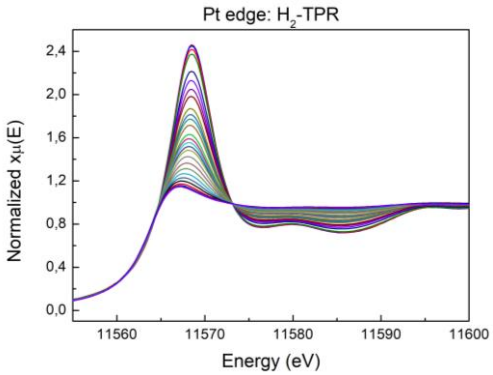

Figure 1: *XANES spectra during H_2-TPR at the Pt-L_{III} edge*

As faster measuring techniques are developed and characterization methods are often combined with each other, the result of one measurement can soon encompass several MB of data. **A Pt and Ga QXAS dataset forms the playground for this thesis.** Data analysis will focus on pre-treatment, adequate comparison and plotting to visualize results, quantification of changes observed and the use of new analysis methods, e.g. statistical techniques like PCA, LCF, …, to get the most out of these data.

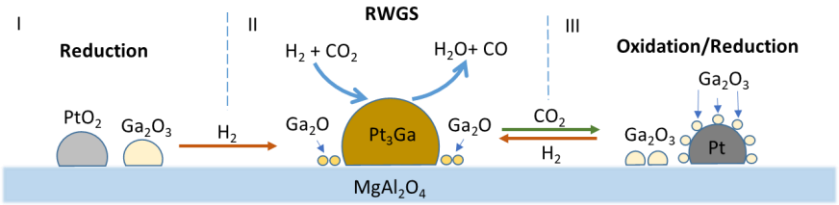

Figure 2: *Schematic representation of surface Pt-Ga alloy formation/segregation expected*

Program

The tasks proposed for this thesis include:

- Literature research on promoted Pt catalysts for propane dehydrogenation
- Theoretical background study on (Q)XAS
- Get familiar with Big Data techniques
- Data treatment, statistical analysis using LCF, PCA, … and interpretation of QXAS spectra.
- Combining and interpreting results.

Joining a XAS campaign at a synchrotron might be possible

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