Case Study

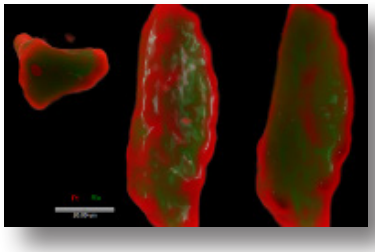
# Chemical tomography: world first in catalysis research

## The Problem

In the chemical industry and industrial research, catalysis plays a vital role. Catalysts are in constant development to fulfil economic, political and environmental demands. Gaining valuable new information about the atomicnanoscale chemical structure, coupled with information about the micro-distribution of such species, has applications across a wide range of disciplines such as materials, biomedical, environmental, and geophysical sciences.

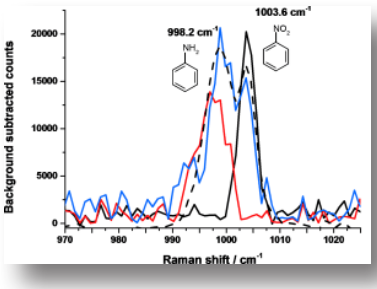
## The Challenge

Determining the active site in a catalyst material and elucidating the related reaction mechanism remain intellectual challenges and are of paramount importance for the rational development of new or better catalysts. Performing a chemical imaging experiment on a solid catalyst catalysing a reaction in the liquid phase has been rarely studied despite its industrial importance - mainly because it is technically challenging.



## The Solution

In the first experiment of its kind, teams from BASF, UCL & Diamond used a combination of microfocus X-ray Fluorescence and X-ray Diffraction Computed Tomography (μ-XRF-CT and μ-XRD-CT) to identify where Pt and Mo Metals are located in NanoSelectTM catalysts. The high brilliance and monochromatic nature of synchrotron X-ray sources are ideal for measurements on samples not only ex situ but also under reaction conditions. In addition to the information gleaned regarding the atomic-nanoscale chemical structure, it is now possible to observe how different preparation methods or deposition sequences affect the micro-distribution of materials, and how structures respond to environmental changes.




## The Benefits

The results have indicated that close contact of these two metals is not needed in order to obtain a high performance and that the active state of the platinum (Pt) catalyst – the structure responsible for the reaction – was dispersed nanoclusters of Pt, and not in crystalline form. This helps to explain not only why the catalyst is so active, but also demonstrated the effectiveness of the method for preparing the catalyst. In terms of catalysis, the formation, phase, and spatial distribution of the active species can be mapped from catalyst preparation, right through to activation, operation, and eventually to deactivation, consequently allowing for a better understanding regarding the correlation of structure and activity.

*"Imaging a working catalyst gives even more information on the exact working mechanism of the metals and stabilizer. For such imaging, it is important to use conditions that are close to the working conditions of a commercial catalyst. These catalysts are most often used in fine chemical applications, which are typically run in liquid phase at mild conditions. The current work shows that the stabilizer is removed from the metal surface under reaction conditions. It is most likely that different results would be obtained if this catalyst were to be imaged under (unrealistic) gas phase conditions."*

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