



Contribution ID: 26

Type: **Oral contribution**

In situ spectroscopy enables the identification of platinum active sites for Water-Gas Shift Reaction

Wednesday, 7 December 2022 14:00 (20 minutes)

Supported metal catalysts for the water-gas shift reaction show strong structure-activity dependence. The direct relationships between spectral features and their function in these catalysts have been challenging to draw, due to the complexity of real catalytic systems. Discussions remain about the nature and reactivity of the active species, whether they are atomically dispersed (AD) or nanoparticles (NP). In this work, we provide an overview of how reactivity correlates with the specific electronic structure/morphology of the supported metal. WGS over Pt/CeO₂ powder catalysts containing AD species and NPs having various diameters in the absence and presence of alkali promoter was monitored by means of in situ ambient pressure X-ray photoelectron spectroscopy (APXPS) and scanning transmission electron microscopy (STEM). Theoretical modelling of platinum NPs arches over spectroscopy and microscopy, thus enables deconvolution of XPS using morphology as a guide. This brings the direct quantification of the different types of platinum sites under working condition. Catalytic tests, carried out in parallel and reproducing the reaction conditions adopted during spectroscopic measurements, provide relevant information about the catalytic performance, thus bridging the pressure gap between techniques.

We show a triangular connection between morphology, electronic structure and performance of actual Pt/CeO₂ catalysts. The apparent activation energy depends negatively on the fraction of corner platinum sites and such dominant active sites are metallic in nature. Other sites (bulk, terrace and edge) on nanoparticles and AD species are spectators. We further predict the intrinsic activation energies of corner sites located at small to large NPs. This work proposes a suitable approach to straightly correlate structure and activity by means of a smart combination of in situ and ex situ characterization techniques with theoretical calculations. The approach is generally applicable and enables the understanding of reaction mechanisms in heterogeneous industrial catalysts.

if "Other", please specify:

I apply for a travel grant

No

Primary author: LI, Xiansheng (ETH Zurich/PSI)

Co-authors: VAN BOKHOVEN, Jeroen A. (ETH Zürich/PSI); ARTIGLIA, Luca (Paul Scherrer Institute)

Presenter: LI, Xiansheng (ETH Zurich/PSI)

Track Classification: Catalysis