Workshop Summary

ALBA II - Workshop on present and future perspectives of catalysis

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Title: *Potential of infrared synchrotron emission spectroscopy for catalysis research*

Short Abstract:
(describe the field, the grand challenge to be solved, the impact if solved; about 2000 character)

Heterogeneous catalysis, which can transform raw materials into valuable chemicals and clean fuels through economically efficient and environmentally friendly processes, has emerged as a field of paramount importance in the modern global economy. Detailed understanding of heterogeneous processes entails knowledge of both the catalyst surface and the reactant-catalyst interface. It is well-known that the surface structure of catalysts is dynamic and often undergoes reconstruction when reactants interact with the outer surface. As a consequence, the application of powerful tools for probing the atomic and molecular species in the topmost layers of solids are under continuous development to refine the understanding of catalysts *in action*. The design of more efficient catalytic materials has benefit of the in-depth characterization of catalyst surfaces by the intensive use of synchrotron radiation that may thoroughly allow the understanding of surfaces and their dynamic evolution during reaction. The unique properties of radiation synchrotron offer new opportunities in diffraction, spectroscopy, small angle scattering or tomographic studies of catalytic materials. Higher detection sensitivity and molecular specificity, faster

acquisition rates, and in-depth information regarding the structure-performance relationship are remarkable among the benefits provided by radiation synchrotron-based techniques. Despite their unique advantages, infrared (IR) synchrotron spectroscopy techniques have not been widely employed by the catalytic community. Herein, it will be presented the potential future directions addressed in the development of infrared spectroscopy exploiting the synchrotron radiation for catalysis studies.

Describe the technique/probe to solve the grand challenge *(about 1500 characters):*

Infrared spectroscopy is a powerful tool that enables direct monitoring of the interaction between adsorbed molecules and the catalyst surface. A large variety of IR techniques (DRIFTS, TIRS, IRES, ATR, IRRAS, etc) can be used in order to obtain information on the surface chemistry of different solids. In all of them, the middle-infrared (MIR) region has been extensively used in catalysis to analyze the chemical species involved in surface reactions. However, the instrumental limitations for routine access to the far-IR (FIR) spectrum have limited the information provided by the vibration energies of the bonds fall in the FIR spectral region such as lattice vibrations, hydrogen bonds, metal-carbon bonds or the skeleton vibration of aromatic molecules. The conventional FIR spectrometers are equipped with a DTGS/Polyethylene detector, whose sensitivity is much lower than that of the MIR spectral detector, and besides the energy of infrared light source is lower in FIR region and the spectral noise is high. By accessing the FIR region insights into the nature of oxide-supported interfaces and surface-adsorbate bonds would be acquired. Highly sensitive microbolometer detectors together with the high photon fluxes provided by synchrotron light allow to overcome the slow response time and limited sensitivity of bolometer-based thermal detectors making widely accessible the FIR region for catalytic, including transient, studies. This, in conjunction with the design of new cells for *in situ* experiments, working at high pressures and temperatures, open new possibilities to expand the potential of MIRAS beamline at ALBA synchrotron in the characterization of catalysts and in the mechanistic study of relevant catalytic processes.

Provide supporting literature, if appropriate or necessary: