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**Doctoral Programme**

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## Guest Lecture

**Title:** "Operando Spectroscopy: The Knowledge Bridge from Fundamental Understanding to Industrial Application"

**Speaker:** Prof. Dr. Miguel Bañares

**Address:** Catalytic Spectroscopy Lab., CSIC-Institute for Catalysis, Madrid, Spain and "Chaire d'excellence" at CNRS-ENSICAen, Caen, France

**Date:** Friday, 18<sup>th</sup> of October 2013

**Time:** 14:30

**Place:** Seminar Room CBEG02 (387, Photonics); Gußhausstraße 27

### Abstract:

Catalysis is at the interface between fundamental science and applied engineering. Catalysis stands on optimization of catalysts, which are essentially nanoscaled materials. Progress in nanomaterials and catalysis stands on three pillars: 1) synthesis of nanomaterials, including the preparation of hierarchically dispersed nano-particles; 2) ab initio studies of materials that enable experimental results to be understood; and 3) advanced, in situ characterization during operation (operando methodology). These three pillars blend for research in catalysis. This approach brings the fundamental insight on the structure-performance relationships of catalysts.

On a second step, it is necessary to translate this knowledge into working catalytic materials to be able to monitor their state in the working state, such as shaped catalysts (e.g., honeycomb catalysts).

I will make a journey bringing catalysis to spectroscopy: from in situ to operando spectroscopic methodologies, what these are and what differentiates them. We will see how operando spectroscopy delivers a direct



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grip on the structural catalysts transformation and how these allows us to understand the catalytic act. Such a model, is further complemented by ab initio studies on the catalyst surface sites and reactivity. This will be illustrated with the case of propane ammoxidation to acrylonitrile on nanoscaled VSbO<sub>4</sub>.

We will also make another journey bringing chemical engineering to operando methodologies, which we will illustrate assessing the role of porosity on a catalyst self-supported wafer used for operando FTIR study of NO<sub>x</sub> selective catalytic reduction.

As a whole, we will present the value of spectroscopy for fundamental and applied understanding, monitoring and catalyst optimization.