Workshop Summary

ALBA II - Workshop on present and future perspectives of catalysis

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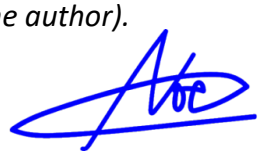

Noelia Barrabés Rabanal

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Speaker *Date*

Speaker and team:

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Title:

Insights in the structure dynamics of cluster heterogeneous catalysts by operando spectroscopy

Short Abstract:

Catalysis is one of the key technologies that may finally enable a truly sustainable society. However, to understand and control catalytic performance of nanoparticles at the molecular level remains a major challenge. Developing novel nanostructures with atomically controlled structural parameters is required, such as the number of atoms (size), elemental composition and surface modification by functional groups. This can be achieved with metal nanoclusters, which have led to advances in nanoscience. The application of monolayer protected metal nanoclusters is arising in several fields other than catalysis, like energy generation, sensing, electronics, bioimaging or medical therapy. Many of them involve the deposition of clusters on solid surfaces (supports), thus preserving the cluster properties is crucial. Particularly in heterogeneous catalysis, atomically precise gold nanoclusters open new opportunities for accurate studies of size-dependent properties, atomic structure effects and reaction mechanisms. However, a fundamental understanding of the cluster-surface interaction, control of the deposition and functionalization still needs to be improved. We shed some light on this by in situ / operando spectroscopic studies (FTIR, XAFS, XPS), indicating a strong influence of the cluster structure/composition and support material on stability and catalytic properties [1-5]. We studied the influence of Au systems, doped with metals such as Co, Ag, Pd, Pt or Cu, tuning the properties and reactivity in several reactions in gas and liquid phase [6-7].

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

Metal nanoclusters with well-defined structure and truly monodisperse purity represents ideal materials for spectroscopic studies. Local structure and electronic state of the clusters, supported or under reaction conditions can be determine by XAS. Some examples were the formation of bimetallic nanoclusters in solution [8], the location of heteroatom metal doping inside the structure [9] or the exact interaction during ligand exchange reactions [10]. Once the cluster are deposited on surfaces, as oxide supports, well-defined heterogeneous catalyst can be prepared. These model catalysts are well suited for fundamental studies of the interrelation of cluster structure, stability, surface sites and catalytic performance. Structure dynamics under reaction conditions were determined by time-resolved measurements, at the laboratory by operando DRIFTS/ATR/FTIR spectroscopy and correlated with operando XAFS at the synchrotron. Complementary characterization by XPS or HRTEM between other techniques were also performed.

Provide supporting literature, if appropriate or necessary:

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