Inorganic Materials & Catalysis
Molecular Heterogeneous Catalysis
Research Project – Emiel Hensen/Valerii Muravev

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NAP-XPS studies over Pd/Ceria model catalysts

Currently, CeO_2 is one the most used materials in catalytic applications. High versatility of its application is provided by unique redox properties, which allow using such materials in wide range of chemical reactions. It is extensively used in environmental catalysis and particularly studied as a component of three-way catalysts (TWC) in combination with precious group metals (i.e. Pt, Rh, Pd). In this respect, CeO_2 appeared to be a perfect candidate as a support for metal nanoparticles, owing to its oxygen storage capacity (OSC) and strong metal-support interaction, which leads to stabilization and high dispersion of active component. Such interaction, as reported previously, leads to atomically dispersed species or so called single-atom catalysts.[1]

Recent work of our group shows that low temperature CO-oxidation can be provided by atomically dispersed Pd-O species on the surface of CeO2 – rods.[2] For further understanding of the nature of species responsible for CO-oxidation over Pd/Ce surfaces, we are aiming to carry out studies of the catalyst's surface under close to reaction conditions using Near-Ambient Pressure X-ray Photoelectron Spectroscopy (NAP-XPS), shown in Fig. 2. This technique coupled with mass-spectroscopy analysis of the gas phase, provides unique information about surface composition and electronic state of species during catalyst's operation. Although most of the NAP-XPS studies are focused on investigation of surface transformations of simplified model catalytic systems, successful attempts on powder samples also have been performed, emphasizing importance of such works from fundamental catalytic as well as spectroscopic points of view.[3]

Main goals of the project are:

- Detailed XPS study and identification of active centres of model and powder Pd/CeO_2 catalysts in atmosphere of reaction mixture ($CO + O_2$, $CH_4 + O_2$)
- Operando XPS – measurements with gas-phase analysis
- Study of $Pd/Ce_{1-x}M_xO_{2-\delta}$ – doped materials (M = Cu, Fe, Mn) with potentially higher oxygen mobility
- Preparation of oriented thin film model system

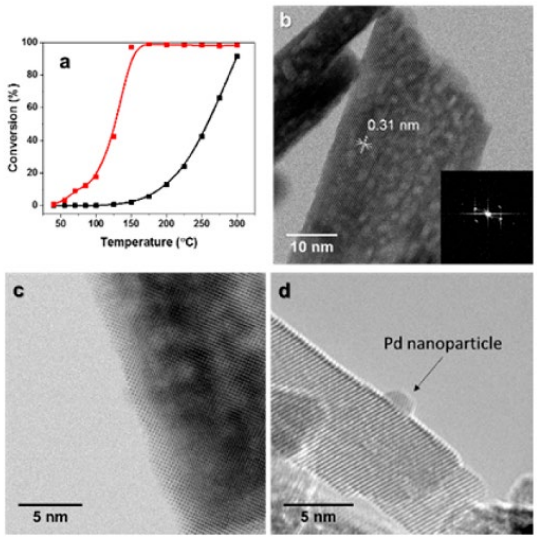

Fig.1 Pd-O single atom species on the (111) proved to be active in low temperature CO oxidation[2]

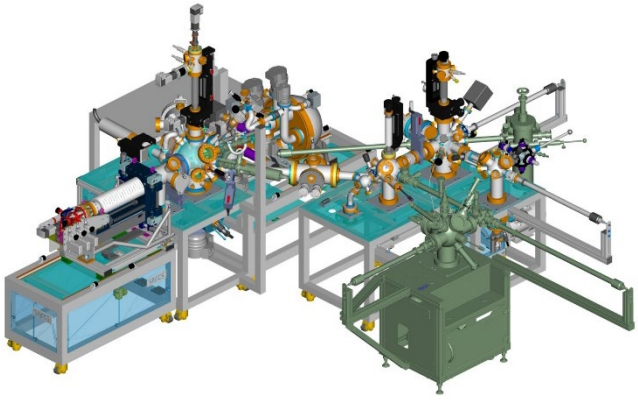

Fig. 2 Lab-based NAP-XPS system

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[2] G. Spezzati, A. Datye, E. Hensen et al., *ACS Catal.*, **2017**, *7*, 6887-6891.
[3] Y. Zhu, L. Nguyen, F. Tao et al., *ACS Catal.*, **2013**, *3*, 2627-2639.