	Experiment title: ZnO-Al_2O_3 catalysts for propane dehydrogenation: correlating structure with catalytic performance	**Experiment number**: MA- 31-01-75
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Report:

The aim of this proposal is to study the structural changes, identify the local coordination and oxidation State of Zn in ZnO/Al_2O_3 and ZnO/SiO_2 catalyst during calcination and propane dehydrogenation. Catalysts prepared by incipient wetness impregnation, Zn-ALD on Al_2O_3, and hydrothermal synthesis were studied. We performed XAFS combined with XRD experiments on the following materials during calcination in air (10 ml/min), ramping from room temperature to 700°C:

1- ZnO deposited on ɔ-Al_2O_3 via ALD (50 ALD cycles): *$ZnO50\_ALD/Al_2O_3$*
2- ZnO and Al_2O_3 deposited on SiO_2 via ALD (50 ALD cycles): *$ZnO50Al_2O_3\_ALD/SiO_2$*
3- ZnO deposited on SiO_2 calcined via ALD (50 ALD cycles): *$ZnO50/SiO_2$*
4- $ZnNO_3$ impregnated on ɔ-Al_2O_3 via incipient wetness impregnation method: *ZnO_WI/Al_2O_3*

The experiments were carried out in a capillary cell (1 mm outer diameter). XAS data were collected in transmission mode. The performed experiments show the crystallization of ZnO and further transformation to $Zn_xAl_yO_z$ (at higher temperatures) for samples deposited/impregnated on ɔ-Al_2O_3. The crystallization temperature and the (local) structure of formed of zinc aluminate depend on the synthesis process: i.e. ALD or incipient wetness impregnation method (Figure 1 and 2).

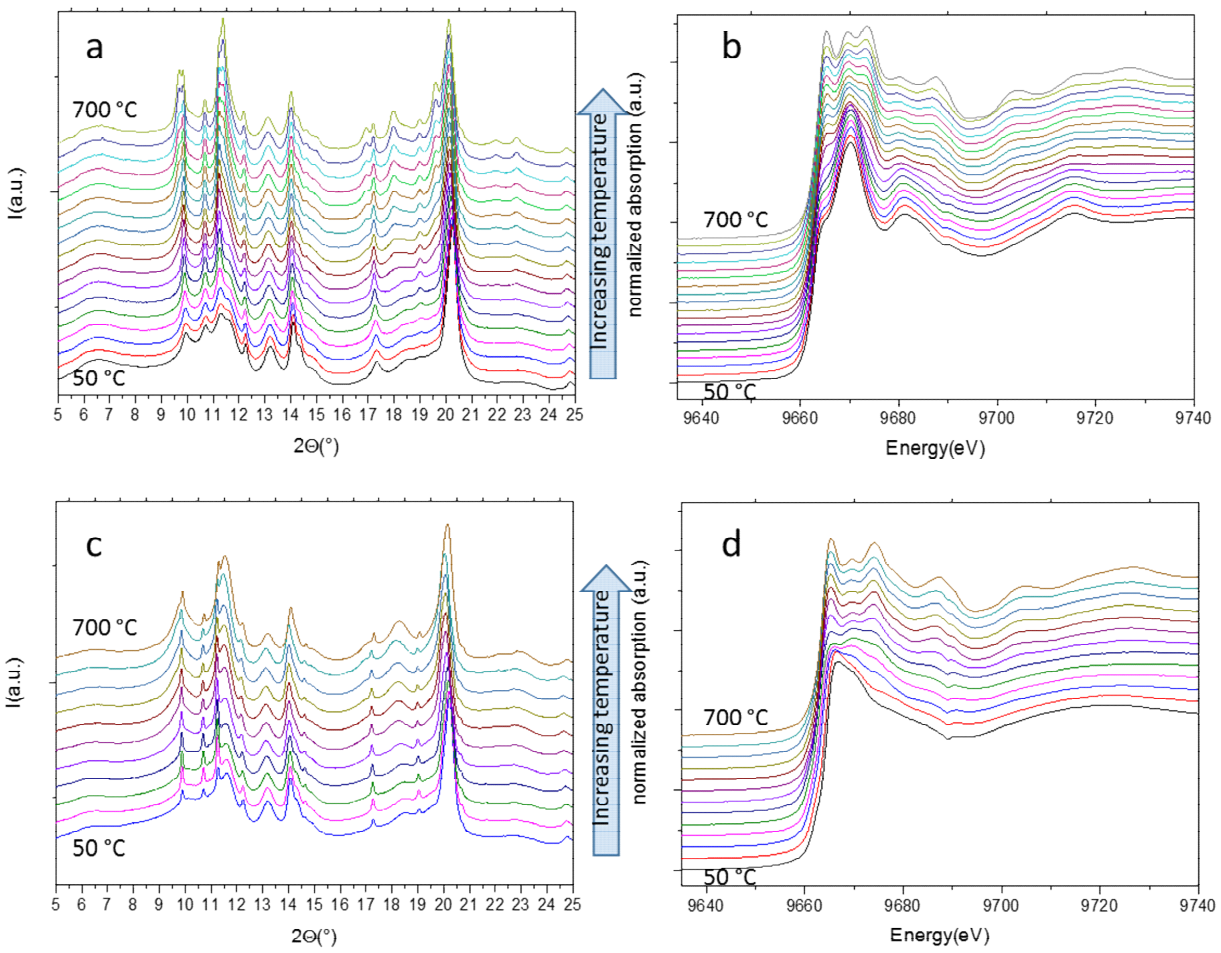

Figure 1: *Consecutive XRD-XANES data collected on ZnO50_ALD/Al_2O_3 (a, b) and ZnO_WI/Al_2O_3 (c,d) during heating in air from room temperature 700°C.*

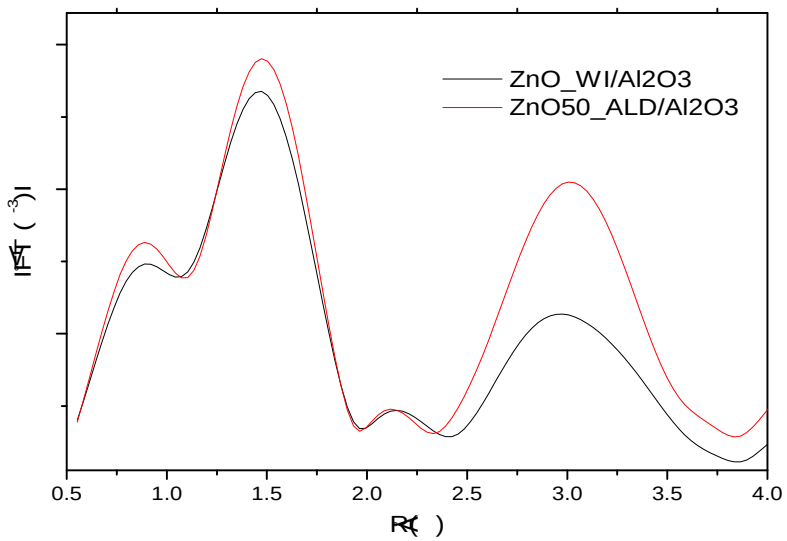

Figure 2: *Fourier transformed EXAFS function for ZnO50_ALD/Al_2O_3 and ZnO_WI/Al_2O_3 after calcination*

Propane dehydrogenation reaction was performed over the materials after calcination at 700°C. A capillary cell was used as reactor. 10 % C_3H_8 in He (10 ml/min) flow was employed for the reaction performed at 600°C. The outlet stream of the reactor was analysed by MS. All the materials with Al_2O_3 support exhibit stable behaviour. On the Other hand, reduction of ZnO is observed on TOS for samples on SiO_2 support. These results correlate with the higher catalytic performance of ZnO/Al_2O_3 with respect to ZnO/SiO_2. Currently data is under analysis and a manuscript is expected to be published based on these results in combination with laboratory techniques analysis within the following months.