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MZrOx (M = Zn, Ga) catalysts for CO2 hydrogenation reaction: exploiting XAS and PXRD to understand catalyst's structure, activity and stability

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In the panorama of CO2 hydrogenation catalysts, the COZMOS project (https://www.aspire2050.eu/cozmos) is investigating MZrO2-x (M : Zn,Ga) as potential catalysts for CO2-to-methanol conversion. Aliovalent elements ZrO2 doping has been largely exploited to improve catalyst's properties through oxygen vacancies (Vo) formation. However, whilst great efforts have been done to improve catalyst performances, very little research investigated how and where the Vo active site was generated during doping. In this contribution, through Powder X-Ray Diffraction (PXRD) and X-Ray Absorption Spectroscopy (XAS) we unveil as two MZrO2-x catalysts having similar catalytic properties are structurally very different. Single phase PXRD patterns are observed for both materials and, as largely accepted, they describe the catalysts as a MZrO2-x solid solutions. Nevertheless, a detailed in-situ - XAS analysis at Zn/Ga/Zr K-edges unveils as: I) ZnZrOx catalyst consists of ZnO nanoclusters embedded in a ZrO2 matrix having catalytic active site at the ZnO/VO/ZrO2 interface and II) Ga substitutionally replaces Zr forming a xGaZr(1-x)ZrZr(2-x/2)OO solid solution where Ga tetrahedral/octahedral coordination changes under reducing conditions increasing the active sites Ga-VO-Zr concentrations. The different structural nature of the two catalysts drastically affects their reactivity and stability. Indeed, whilst any evident differences are observed for GaZrOx after reaction, ZnO/ZrO2 report-significant variations of Zn total concentration and local environment. By in-situ PXRD and ex-situ XAS we observe as during H2 activation ZnO cluster dimension increases favouring Zn sublimation, globally causing a drastic loss of active ZnO/ZrO2 interface and reducing tetragonal ZrO2 polymorph stability.

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