ARTICLE

Received 00th January 20xx, Accepted 00th January 20xx

DOI: 10.1039/x0xx00000x

Morphology-electronic effects in *ultra*-model nanocatalysts under CO oxidation reaction: the case of ZnO ultrathin films grown on Pt(111)

Hang Liu,^a Lei Zhang,^a Sébastien Lebègue,^b Fabrice Bournel,^{a,c} Jean-Jacques Gallet,^{a,c} and Ahmed Naitabdi^a*

Supplementary Information:

The Supplementary Information provide two additional figures to the main manuscript. The first, Figure S1, shows Low-Energy Electron Diffraction (LEED) patterns that were obtained for the ZnO film grown on Pt(111) with a thickness of 1 ML as a function of the treatment ($(O_2 + CO)$ exposure and temperature). These patterns are directly related to Figure 5 in Section B of the main manuscript, as they were acquired on the same 1 ML sample.

The second, Figure S2, corresponds to STM images and related LEED patterns acquired on the ZnO film grown on Pt(111) with a thickness of 2 ML as a function of the treatment ($(O_2 + CO)$ exposure and temperature).

The third, Figure S3, corresponds to XPS core level spectra acquired in the binding energy interval of the Zn 3p as prepared in UHV and under (CO+O2) as a function of stepwise annealing from room temperature up to 485 K.

This Supplementary Information document provides also the link to the author's webpage for additional resources.



^{a.} Sorbonne Université, CNRS, Laboratoire de Chimie Physique Matière et

Rayonnement, UMR 7614, 4 place Jussieu, 75005 Paris, France.

^{b.} Université de Lorraine, CNRS, Laboratoire de Physique et Chimie Théoriques, UMR 7019, 54000 Nancy.

^c Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, 91192 Gif sur Yvette, France.

^{*}Corresponding author: ahmed.nait_abdi@sorbonne-universite.fr Electronic Supplementary Information (ESI) available: See DOI: 10.1039/x0xx00000x

ARTICLE

Figure S1: LEED patterns of ZnO film grown on Pt(111) with 1 ML in thickness as a function of the treatment, and corresponding to the sample shown in the Figure 5 of the manuscript. (a) LEED pattern (electron energy 45.3 eV) of the as-grown ZnO film. (b) (electron energy 47.8 eV) LEED pattern of the same sample as in (a) after exposure to the (O_2 :CO) mixture at 1 mbar at room temperature. (c) LEED pattern (electron energy 48 eV) of the same sample as in (b) after subsequent exposure to (O_2 :CO) mixture at 1 mbar at 440 K.



Figure S2: (a) STM image ($V_{bias} = 2.6 V$, $I_{set} = 190 pA$) of the as-grown ZnO film on Pt(111) at a thickness of 2 ML. (b) STM image (2.4 V, 190 pA), of the same sample as in (a), after exposure to the (O_2 :CO) mixture (4:1) under 1 mbar of total pressure at room temperature. (c) STM image (0.8 V, 100 pA), of the same sample as in (b), after annealing at 440 K under (O_2 :CO) mixture (4:1) at 1 mbar. (a') (electron energy 62 eV), (b') (electron energy 61.8 eV), and (c') (electron energy 66.8 eV) are LEED patterns corresponding the samples shown in (a), (b) and (c), respectively.

ARTICLE



Figure S3: In situ high resolution XPS core level spectra of Zn 3p with deconvolution components of a ZnO ultrathin film on Pt(111) with a thickness of 1 ML acquired a a photon energy of hv = 165 eV as prepared (UHV) at room temperature and in situ under 1 mbar of (CO+O2) as function of the temperature from RT up to 485 K.

This Supplementary Information document provides also the link to the author's webpage for additional resources.

Ahmed NAÏTABDI's Webpage at Sorbonne Université: https://lcpmr.cnrs.fr/content/ahmed-naitabdi