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Supporting Information

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Calcium Oxide Supported on Monoclinic Zirconia as a Highly Active Solid Base Catalyst

Anne Mette Frey, Tomas van Haasterecht, Krijn P. de Jong, and Johannes Hendrik Bitter*[a]

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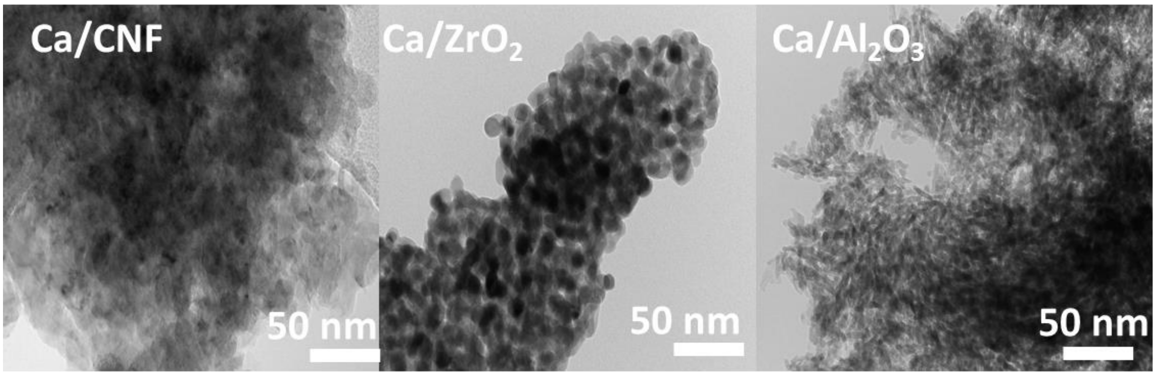

Figure S1. TEM images of CaO/CNF-600, CaO/ZrO_2-600 and CaO/Al_2O_3-600. On CNF CaO particles of ~ 3 nm were well-distributed over the support. For CaO/ZrO_2-600 and CaO/Al_2O_3-600 no CaO particles were observed. This indicates that the CaO is either very well dispersed i.e. a film is formed or CaO is incorporated in the support (i.e. interlayer or solid solution).

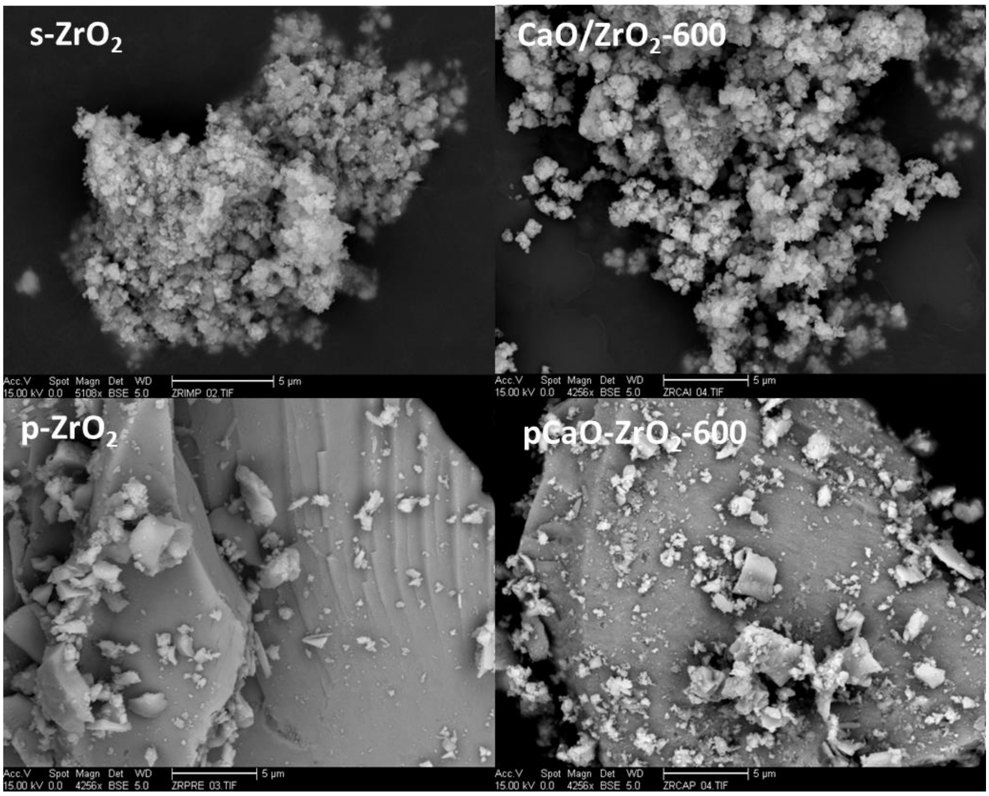

Figure S2. SEM of m-ZrO_2, t-ZrO_2 and CaO/ZrO_2-600 and p-CaO-ZrO_2-600

All Ca-containing samples displayed similar morphologies as the bare supports.

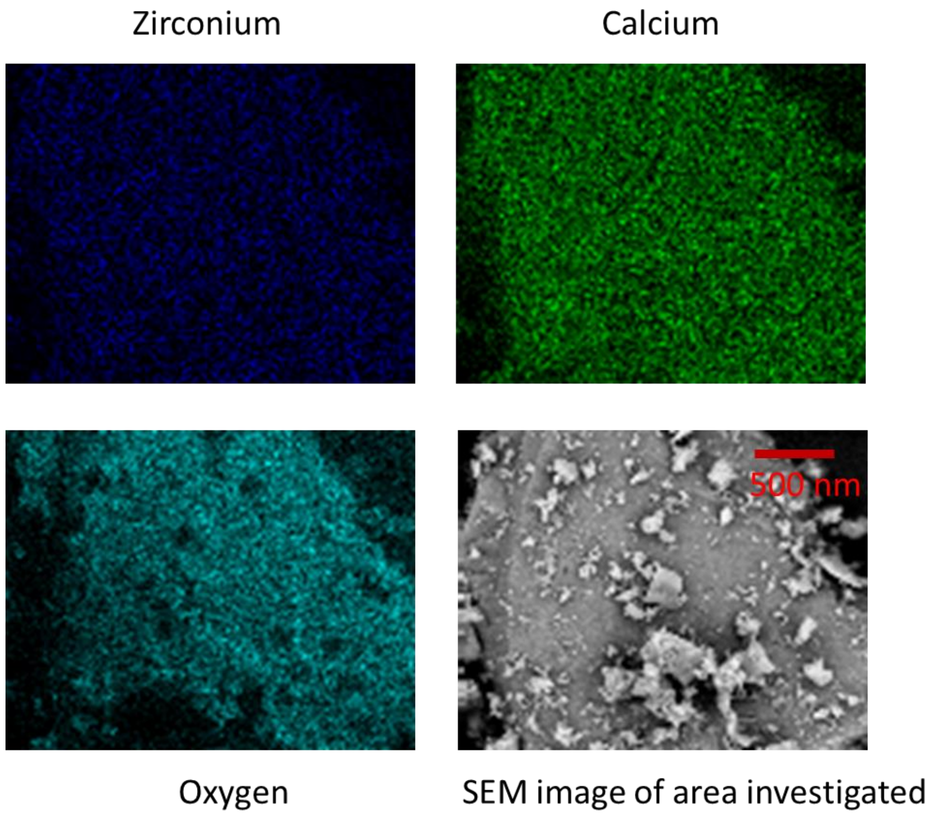

Figure S3. SEM and element mapping of p-CaO-ZrO_2-800 showing a homogeneous distribution of Ca and Zr.

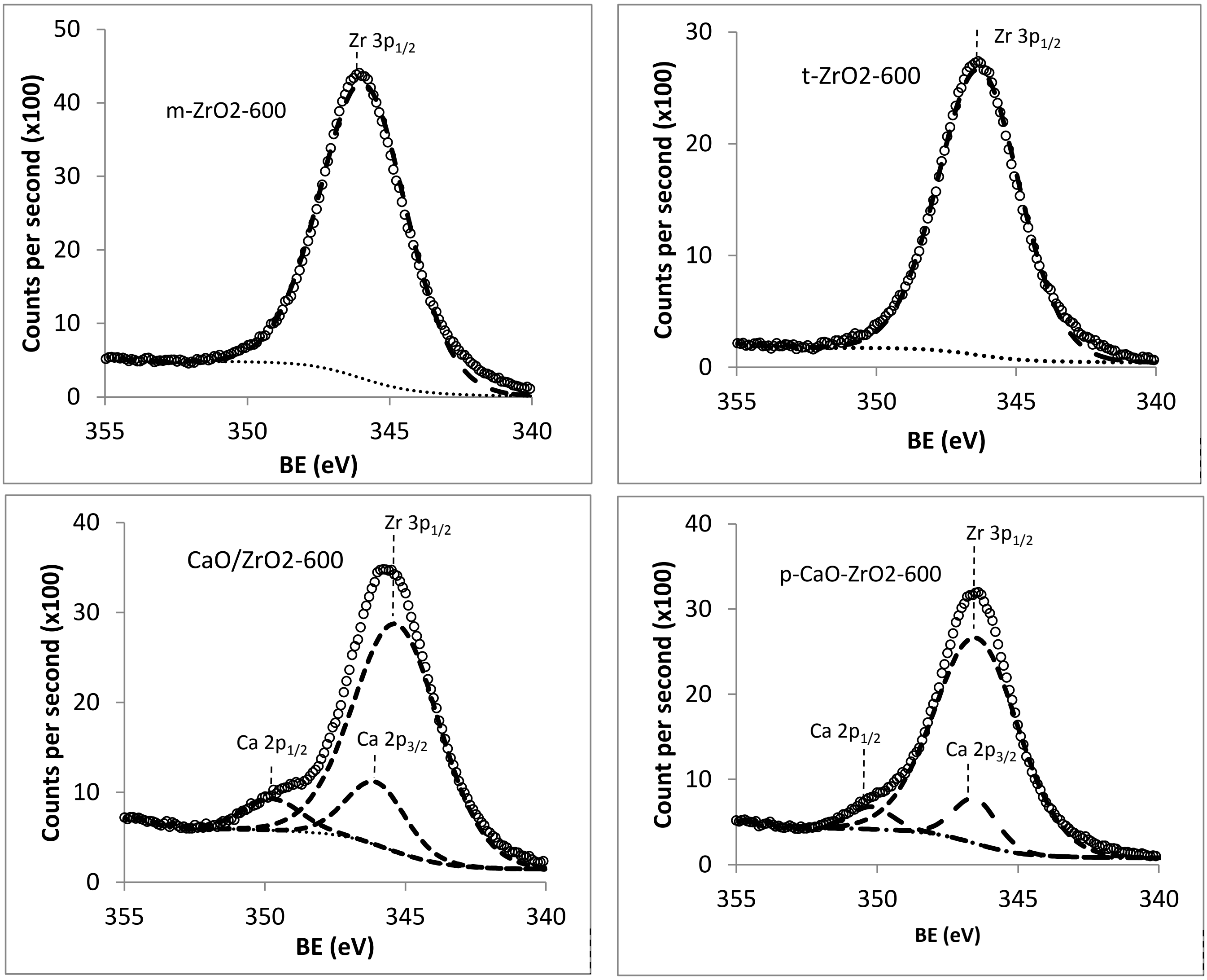

Figure S4. XPS region scans and fitted contribution of Ca2$p_{1/2}$, Ca2$p_{2/3}$ and Zr3$p_{1/2}$.

Figure S4 shows the X-ray photoelectron spectra of the Ca 2p and Zr 3$p_{1/2}$ core levels of the impregnated (Ca/ZrO_2-600) and precipitated (p-CaO-ZrO_2-600) samples. The Ca 2$p_{1/2}$ BE of CaO is reported to be located at 349.7 with a relative difference of 3.7 eV between 2$p_{1/2}$ and 2$p_{2/3}$ [1]. A distinguished valley should exist between the Ca2$p_{1/2}$ and the Ca2$p_{2/3}$ contributions however analysis is complicated by the overlap of the Ca 2p doublet with the Zr 3p ½ photospectric contribution. Therefore we also show the Zr 3$p_{½}$ contributions of the zirconia supports (m-ZrO2-600 and t-ZrO2-600).

The areas of each contribution were then computed using CASA XPS by fitting the experimental spectra to Gaussian/Lorenztian curves (GL30) after removal of the background (Shirley function). The Ca/Zr atomic ratio's where calculated from the areas of each component using Scofield relative sensitivity factors resulting in a Ca/Zr ratio of 0.29 for Ca/ZrO_2-600 and a Ca/Zr ratio of 0.17 for p-CaO-ZrO_2-600.

[1] Sosulnikov et al.- Journal of Electron Spectroscopy and Related Phenomena, 59, 1992, 111-126