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Supplementary Information

Unravelling the nature, evolution and spatial gradients of active species and active sites in the catalyst bed of unpromoted and K/Ba-promoted Cu/Al_2O_3during CO_2 capture-reduction

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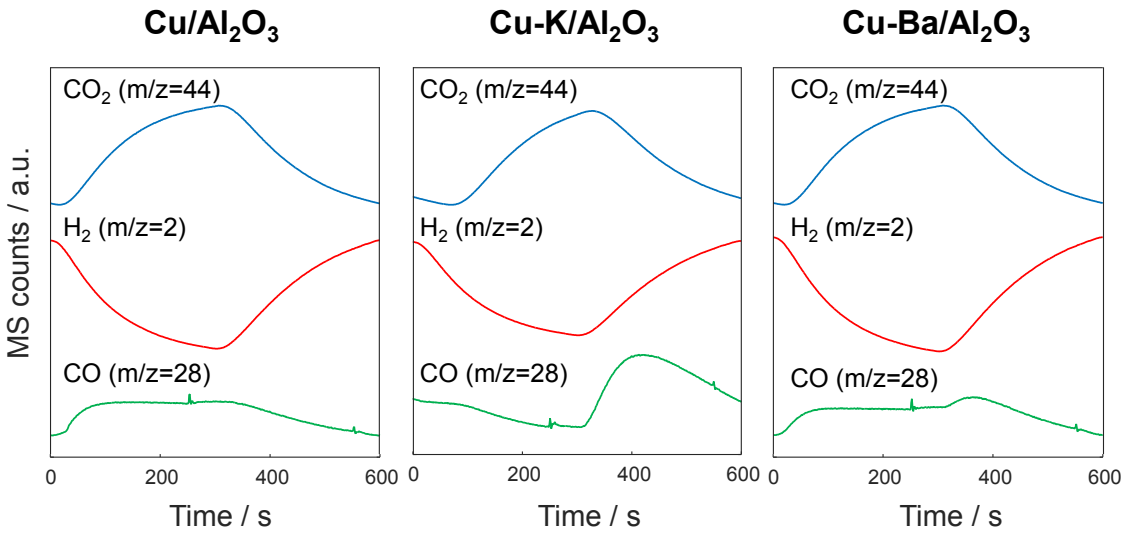

Figure S1. Concentration profiles of CO_2, H_2, and CO measured by mass spectrometry during XAFS and XRD measurements using the capillary reactor under CCR condition (1 vol% CO_2 in He vs. 100 vol% H_2, both at 4.5 NmL/min and for 300 s thus 600 s of one CCR cycle at 350 °C). CO concentration was determined from m/z=28 by subtracting the contribution of CO_2 to the m/z.

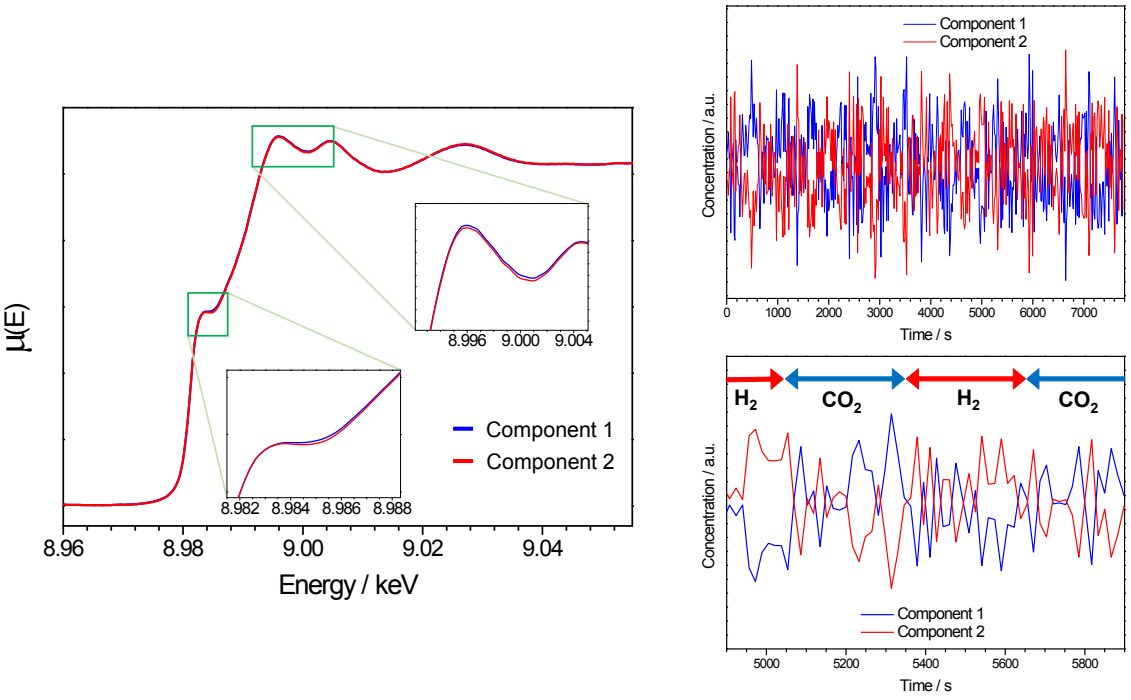

Figure S2. (left) Component XAFS spectra for Cu/Al_2O_3 at the back position during 13 CCR cycles extracted after MCR and (right, top) corresponding component concentration profiles with (right, bottom) a selected region to show the relation between the gas atmosphere in the capillary reactor and the concentration responses of the two spectral components. The experimental conditions are shown in the caption of Figure S1.

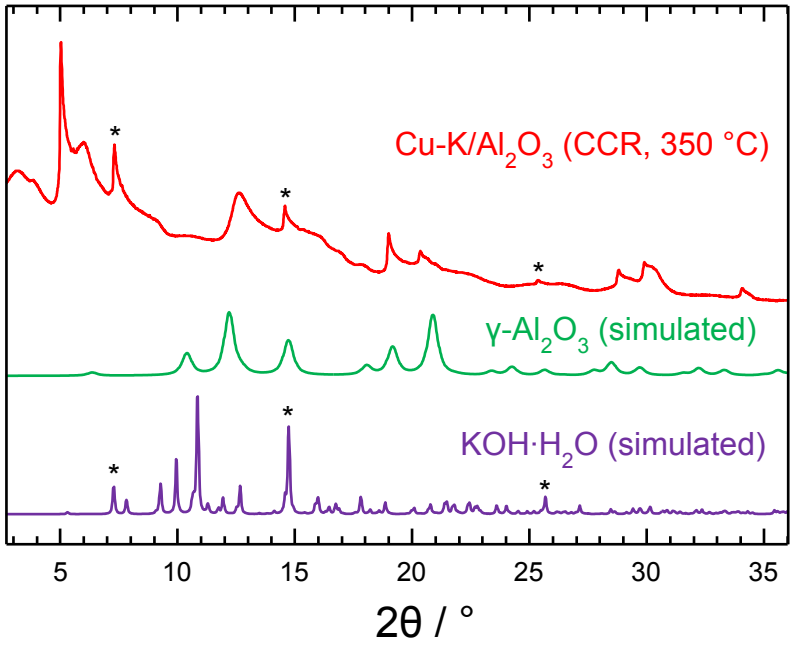

Figure S3. Averaged XRD pattern of Cu-K/Al_2O_3 during CCR and simulated patterns of γ–Al_2O_3 (COD: 1531489, FWHM = 0.5°) and KOH·H_2O (COD: 1528416, FWHM = 0.1°).