Supplementary Information

Correlating spatially resolved catalysis and Raman spectroscopy during CO oxidation over Cu/CeO_2 catalysts

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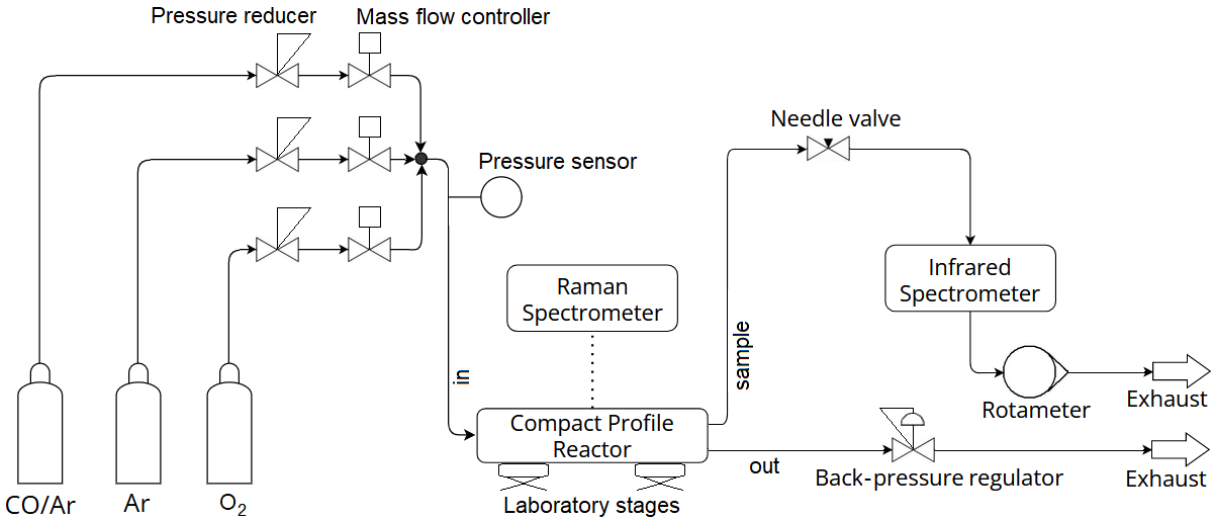

Figure S1 Scheme of the experimental setup, showing the coupling of the compact profile reactor to the gas supply, Raman and IR spectrometer. A small fraction of the gas feed was sampled through the capillary and send to the IR spectrometer for quantitative analysis ('sample'). Raman spectra were taken at 632.8 nm laser excitation. For a detailed description see also manuscript.

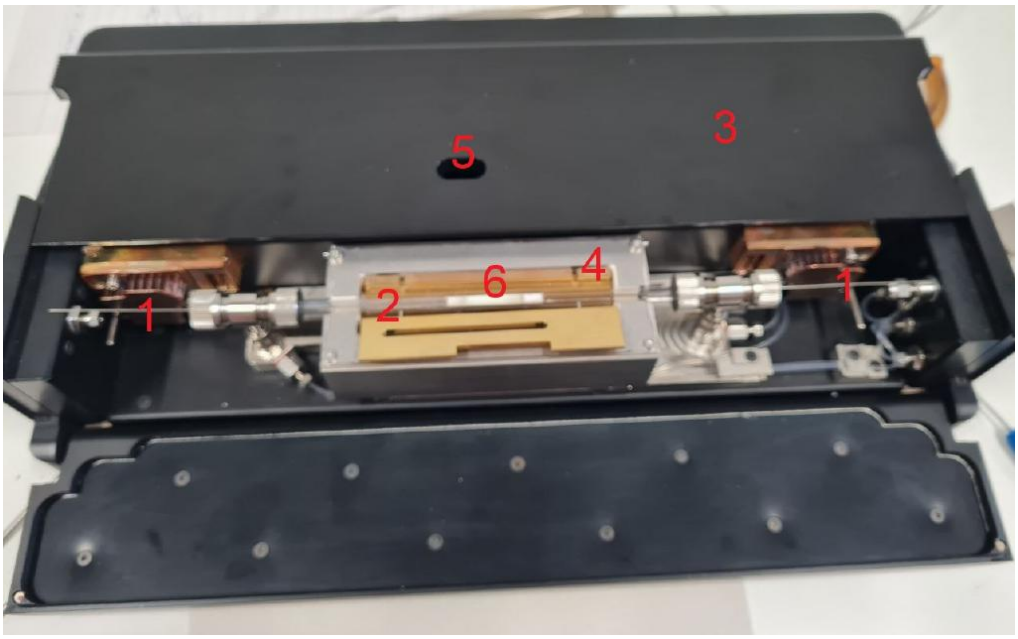

Figure S2 Opened compact profile reactor with the sampling capillary (1) traversing the reactor tube (2). The capillary and reactor tube are enclosed by the reactor housing (3). The reactor tube is embedded in the heating block (4) and can be moved with respect to the sampling capillary. The window (5) in the reactor housing allows for spectroscopic analysis.

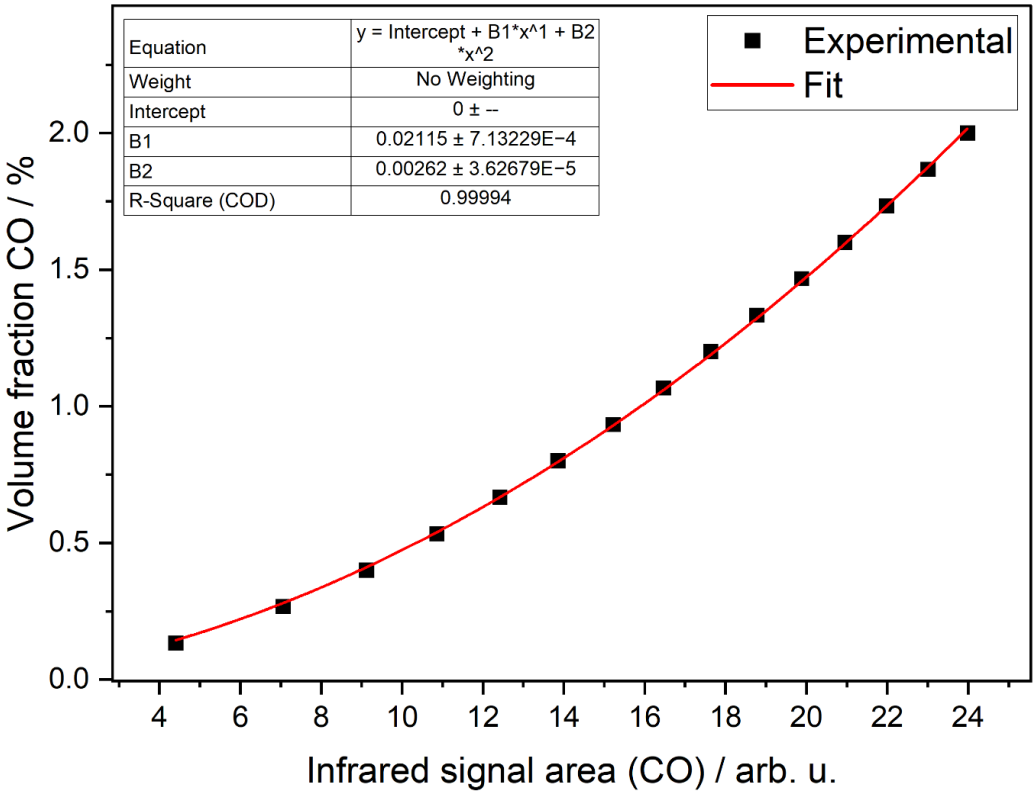

Figure S3 Volume fraction of CO as a function of the area of the infrared CO signal, used as calibration curve.

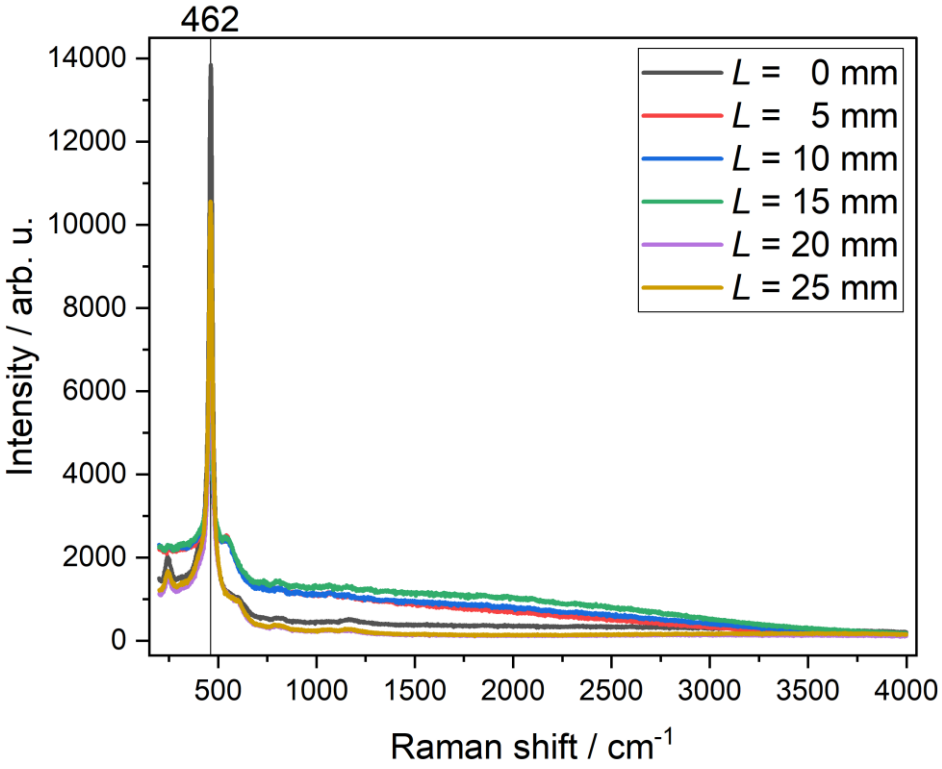

Figure S4 Raw Raman spectra at 632.8 nm excitation of 0.38 wt% Cu/CeO_2 with an average catalyst bed density of 14.36 mg/mm during CO oxidation (2 vol% CO/1 vol% O_2/Ar) at a total flow rate of $\dot{V}_{tot}$ = 150 mL min^{-1} and a pressure of 1 bar (sampling flow rate: 8.7 mL min^{-1} to 8.2 mL min^{-1}) for different positions *L* within the catalyst bed.

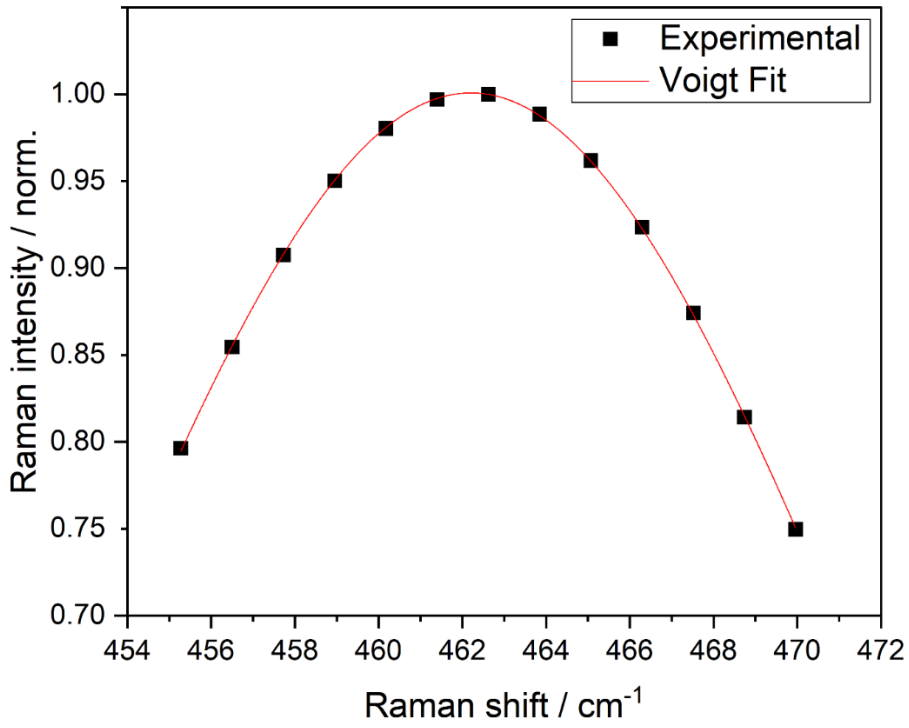

Figure S5 Voigt fit for determination of the position of the F_{2g} signal of 0.38 wt% Cu/CeO_2 during CO oxidation at position 20 (average catalyst bed density: 14.36 mg mm^{-1}). Reaction conditions: 2 vol% CO/ 1 vol% O_2/Ar, total flow rate: $\dot{V}_{tot}$ = 150 mL min^{-1}, pressure: 1 bar, sampling flow rate: 8.7 mL min^{-1} to 8.2 mL min^{-1}.

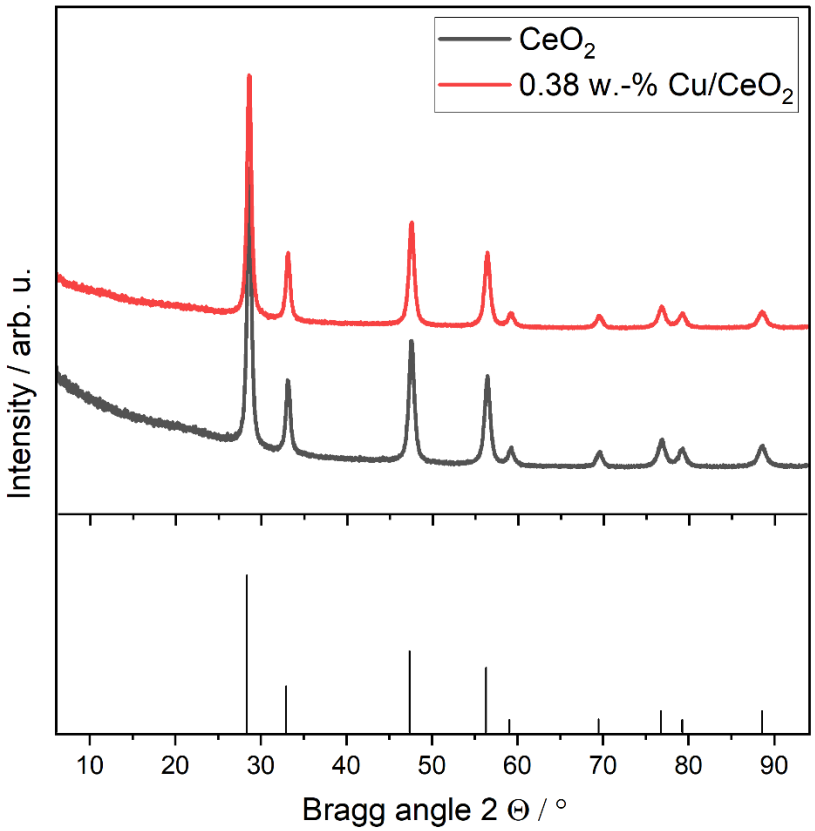

Figure S6 X-ray diffractograms of CeO_2 and 0.38 wt% Cu/CeO_2 measured as prepared, offset for clarity (upper panel), and compared to the JCPDS card number 34-0394 of CeO_2 (lower panel).

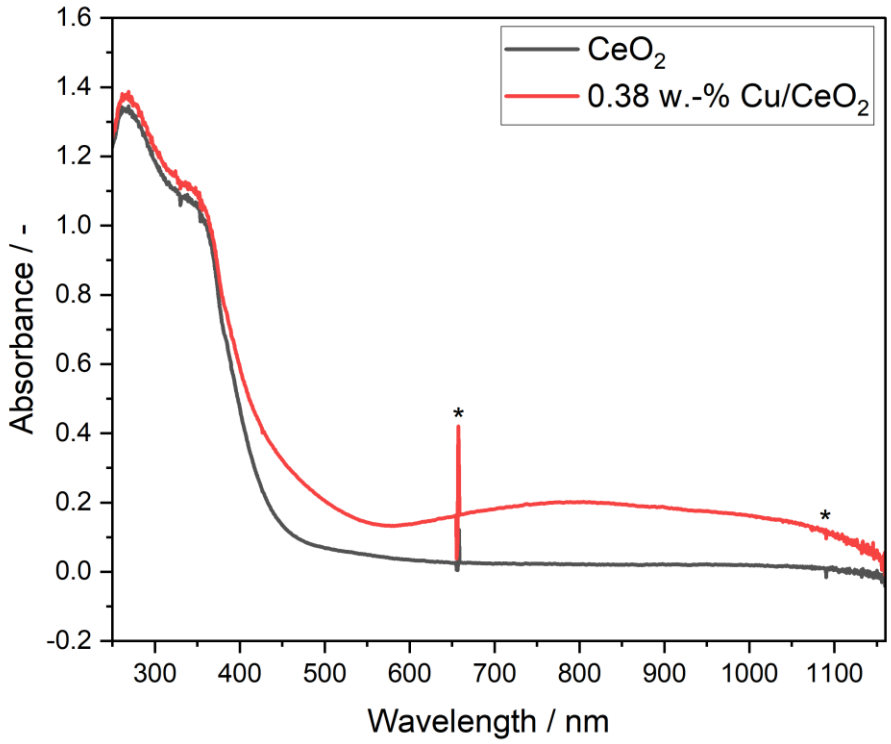

Figure S7 UV-vis spectra of CeO_2 and 0.38 wt% Cu/CeO_2 measured as prepared. Signals marked with * are artefacts from the measurement, caused by the spectrometer.

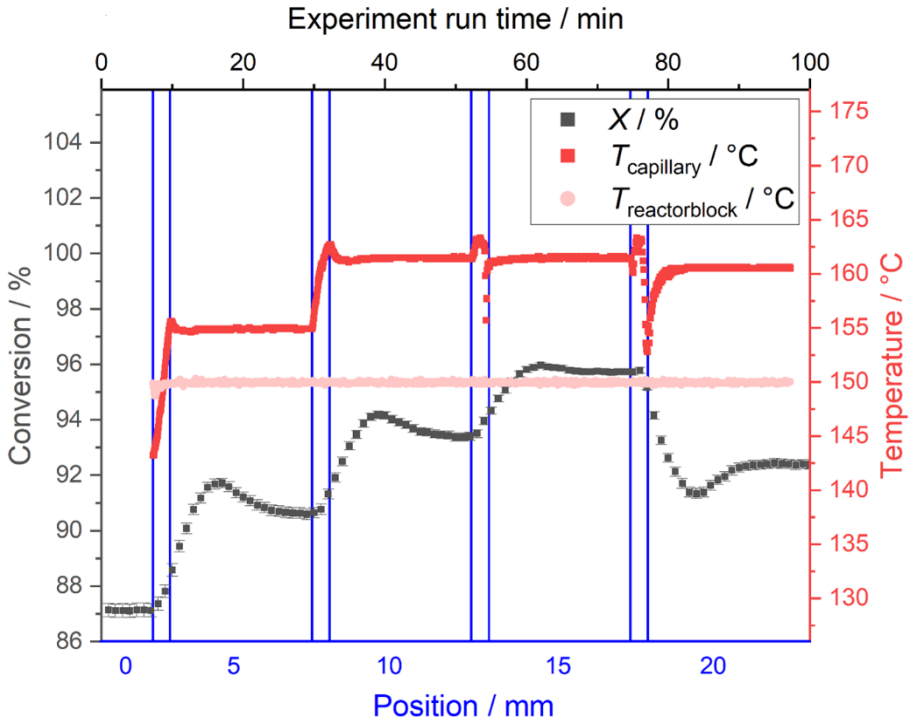

Figure S8 Conversion and temperature as a function of experiment run time and position within the catalyst bed for 0.38 wt% Cu/CeO_2 (509 mg; average catalyst bed density: 15.42 mg/mm) during CO oxidation (2 vol% CO/1 vol% O_2/Ar) at a total flow rate of $\dot{V}_{tot}$ = 150 mL min^{-1}. The pressure downstream of the catalyst bed was 1 bar and the pressure upstream was 4 bar (sampling flow rate: 4.5 mL min^{-1} to 4.1 mL min^{-1}).

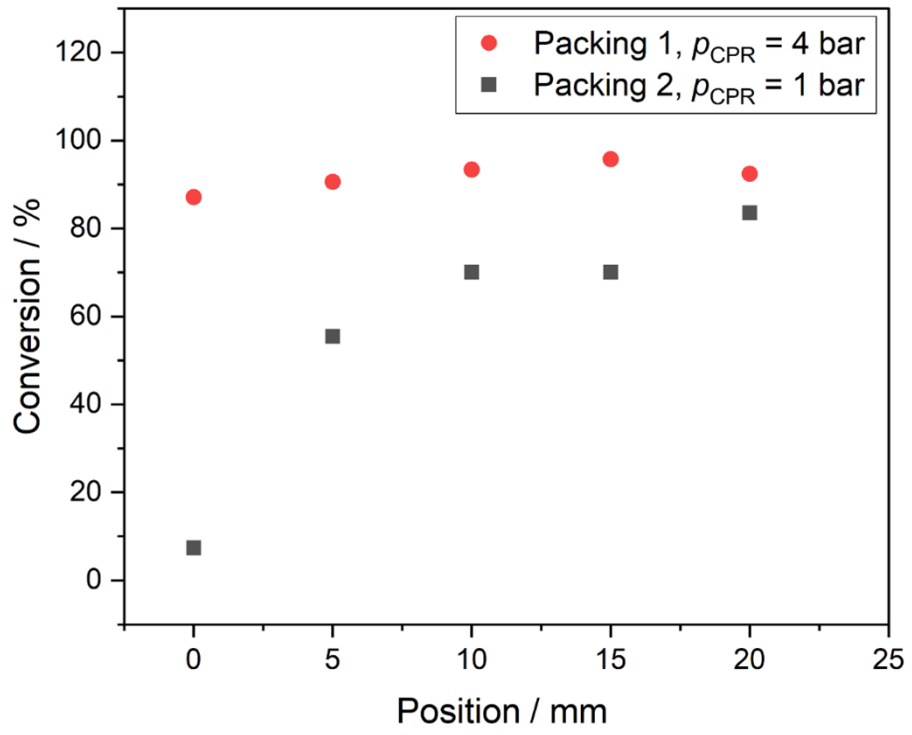

Figure S9 Conversion as a function of position within the catalyst bed for 0.38 wt% Cu/CeO_2, during CO oxidation (total flow rate: $\dot{V}_{tot}$ = 150 mL/min, 2 vol% CO/1 vol% O_2/Ar, $T_{reactor}$ = 150 °C, p_{BPR} = 1 bar) for different packings (packing 1: 15.42 mg/mm, packing 2: 14.36 mg/mm.).

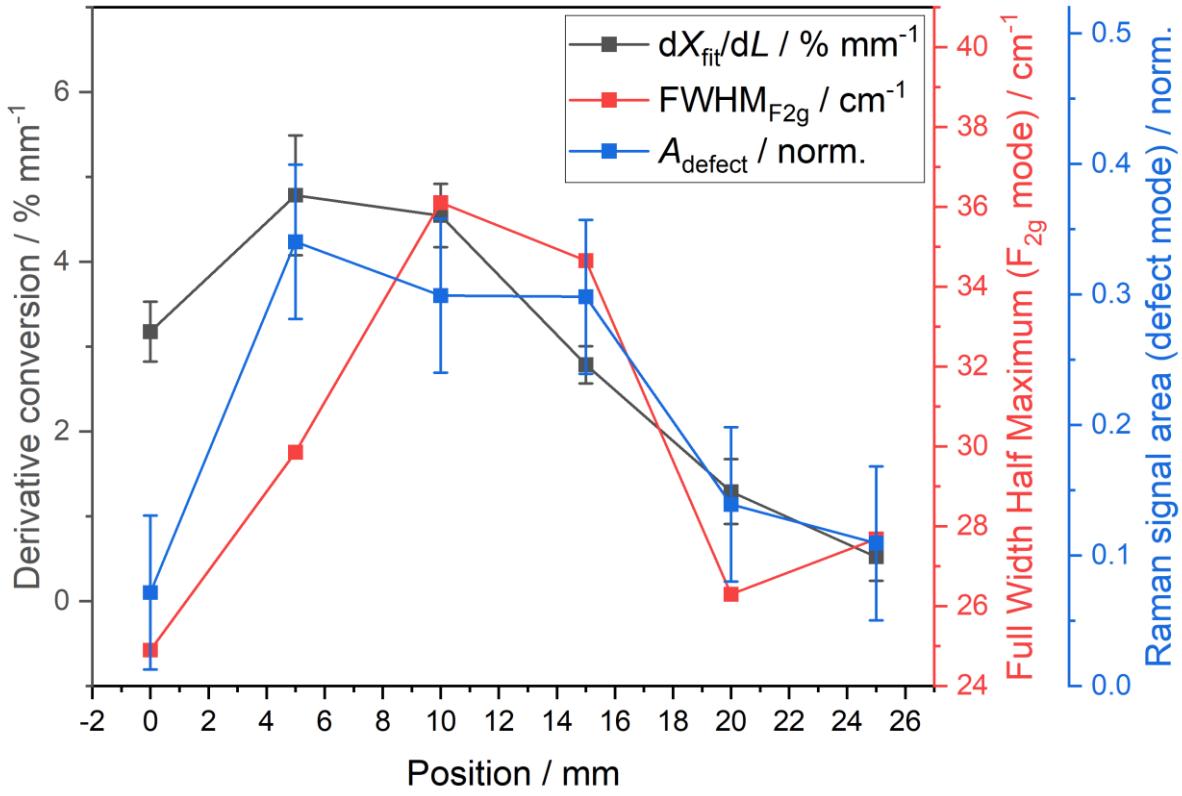

Figure S10 Correlation of spatially resolved catalytic and Raman spectroscopic results during CO oxidation over 0.38 wt% Cu/CeO_2. Shown are the derivative conversions, the FWHM of the F_{2g} mode $\tilde{\upsilon}_{F2g}$ and the area of the defect mode A_{defect} as a function of the position with the catalyst bed. Reaction conditions: 2 vol% CO/1 vol.-% O_2/Ar, total flow rate $\dot{V}_{tot}$ = 150 mL min^{-1}, pressure: 1 bar, sampling flow rate: 8.7 mL min^{-1} to 8.2 mL min^{-1}.