

## Supporting Information

Elucidating Active CO-Au Species on Au/CeO<sub>2</sub>(111):

A Combined Modulation Excitation DRIFTS and

Density Functional Theory Study

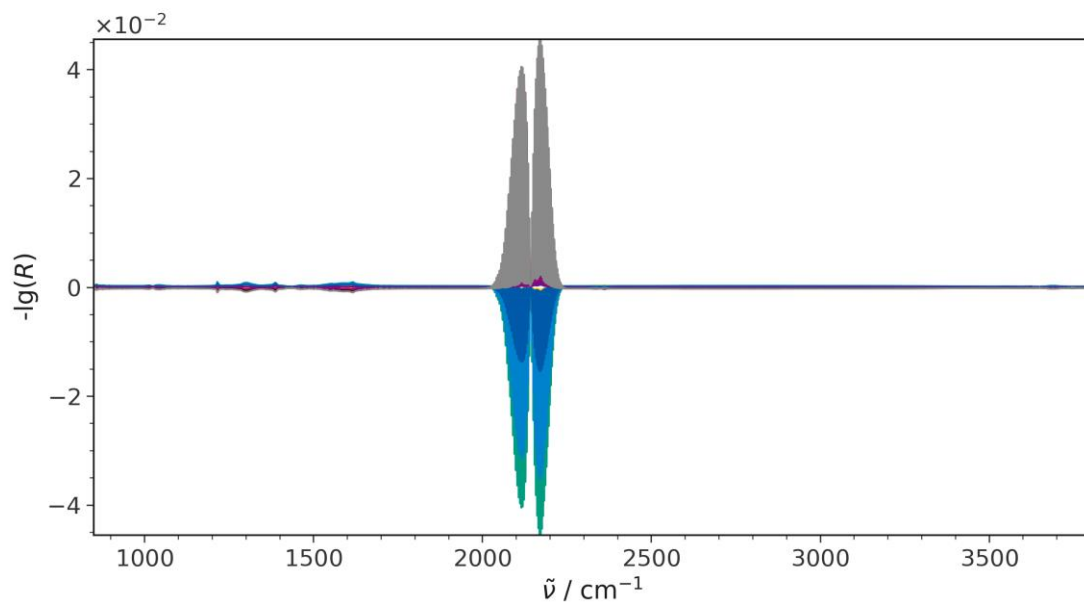
Jakob Weyel<sup>†</sup>, Marc Ziemba<sup>†</sup>, Christian Hess<sup>\*</sup>

Eduard-Zintl-Institute of Inorganic and Physical Chemistry, Technical University of Darmstadt,  
Alarich-Weiss-Str. 8, 64287 Darmstadt, Germany

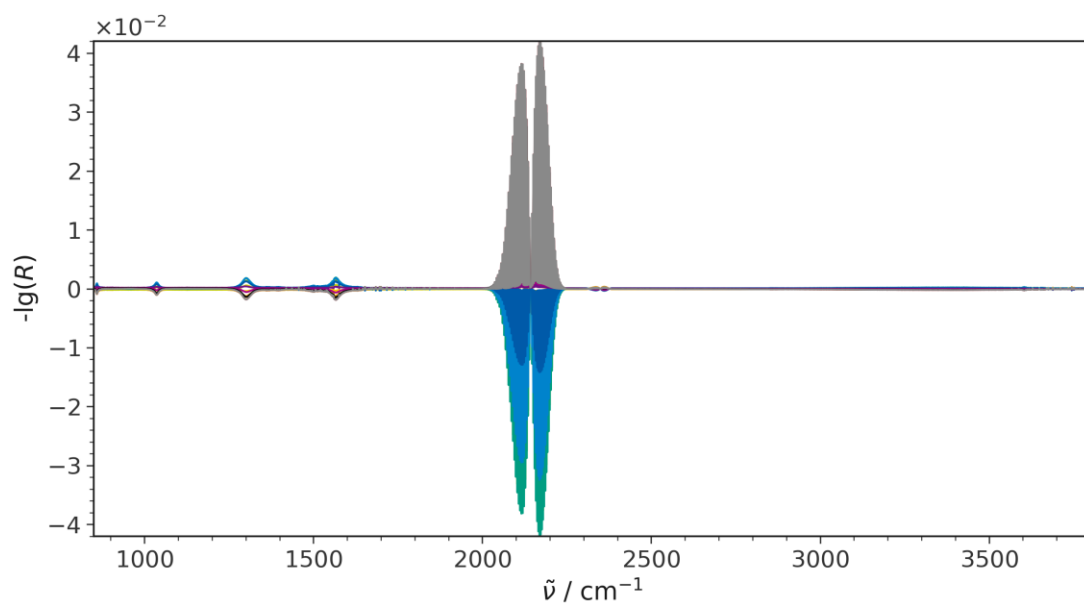
\*email: christian.hess@tu-darmstadt.de

<sup>†</sup>Both authors contributed equally

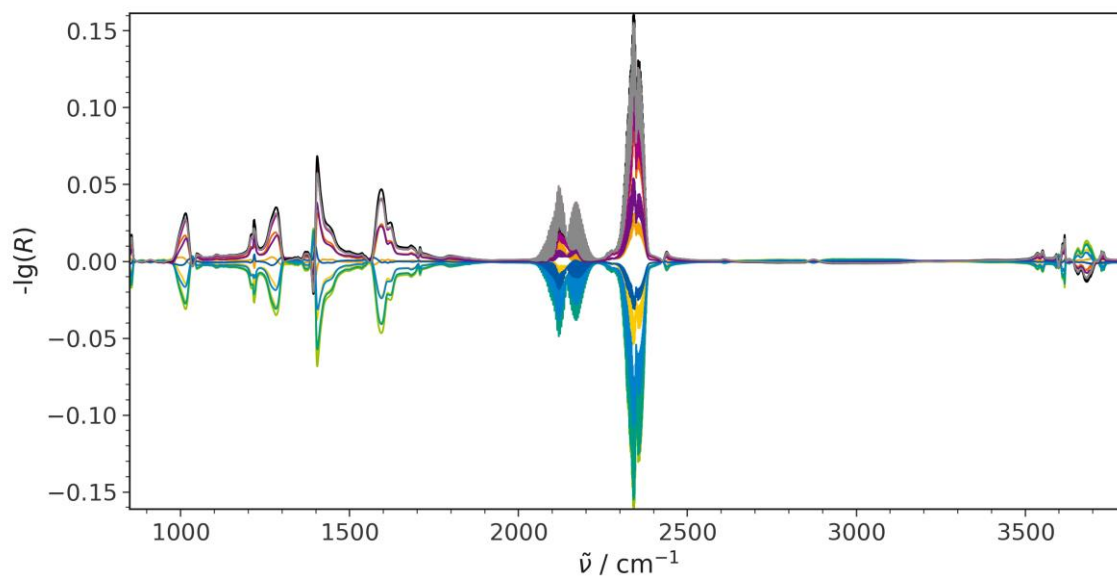
## ME-DRIFTS



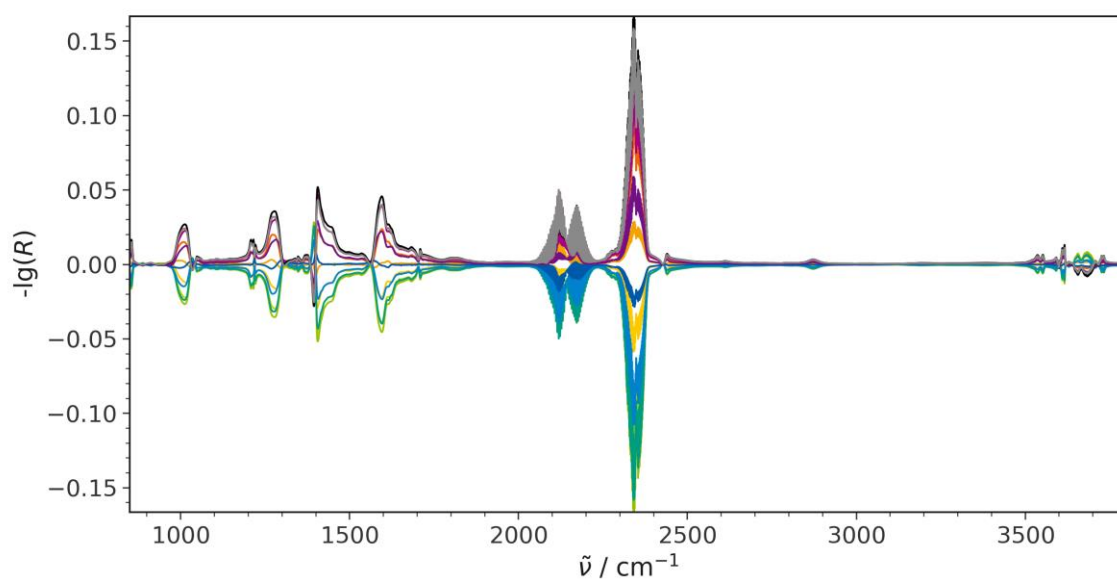
**Fig. S1:** PSD spectra of the entire spectral range of CeO<sub>2</sub> sheets.



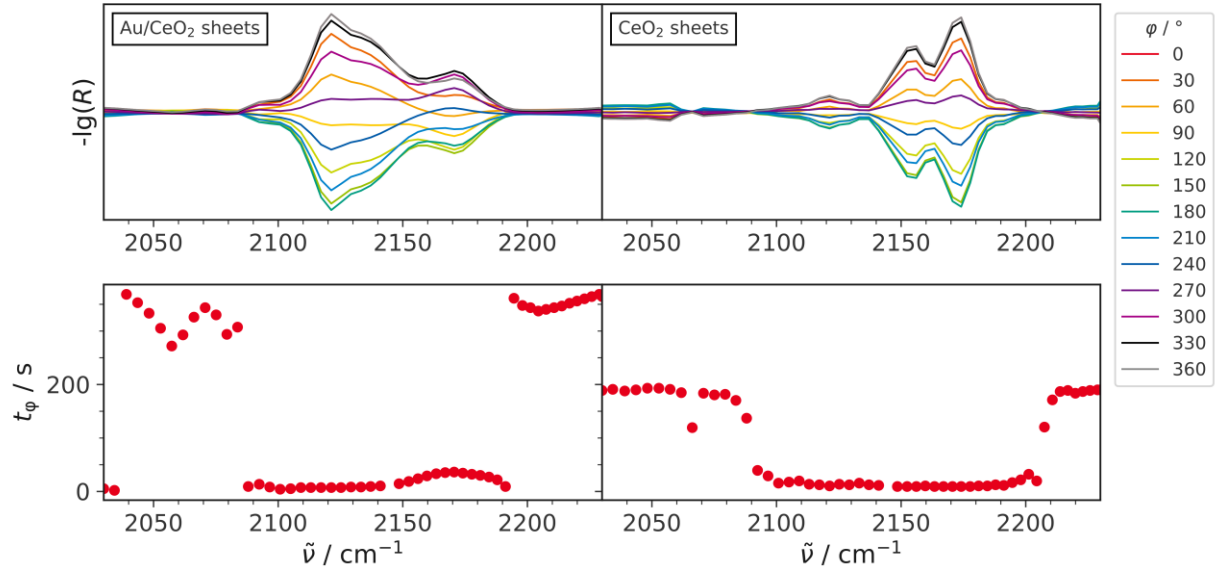
**Fig. S2:** PSD spectra of the entire spectral range of CeO<sub>2</sub> polyhedra.



**Fig. S3:** PSD spectra of the entire spectral range of Au/CeO<sub>2</sub> sheets.



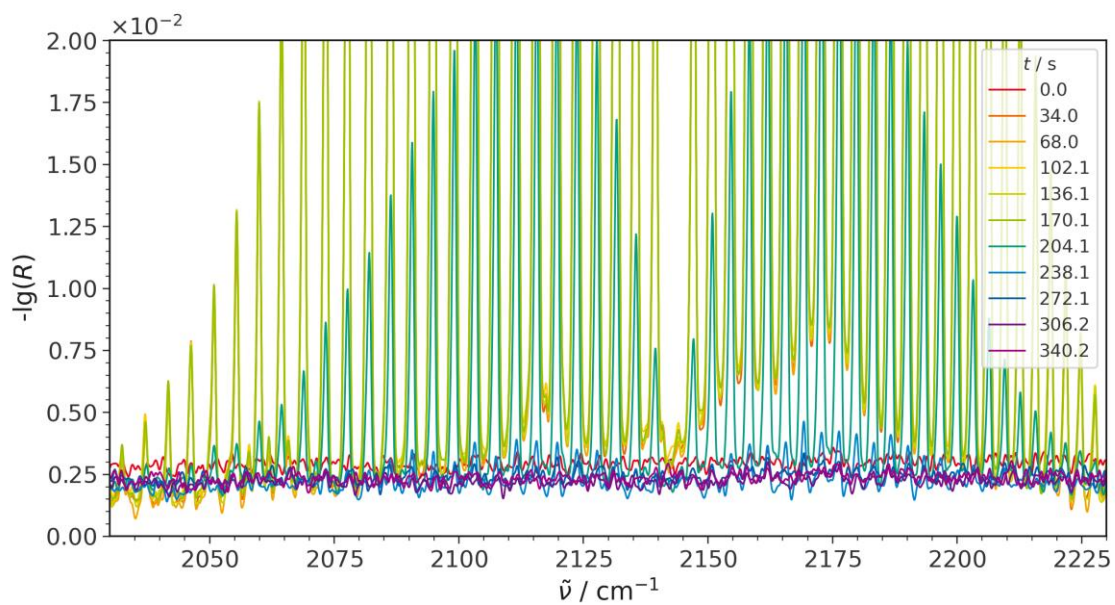
**Fig. S4:** PSD spectra of the entire spectral range of Au/CeO<sub>2</sub> polyhedra.



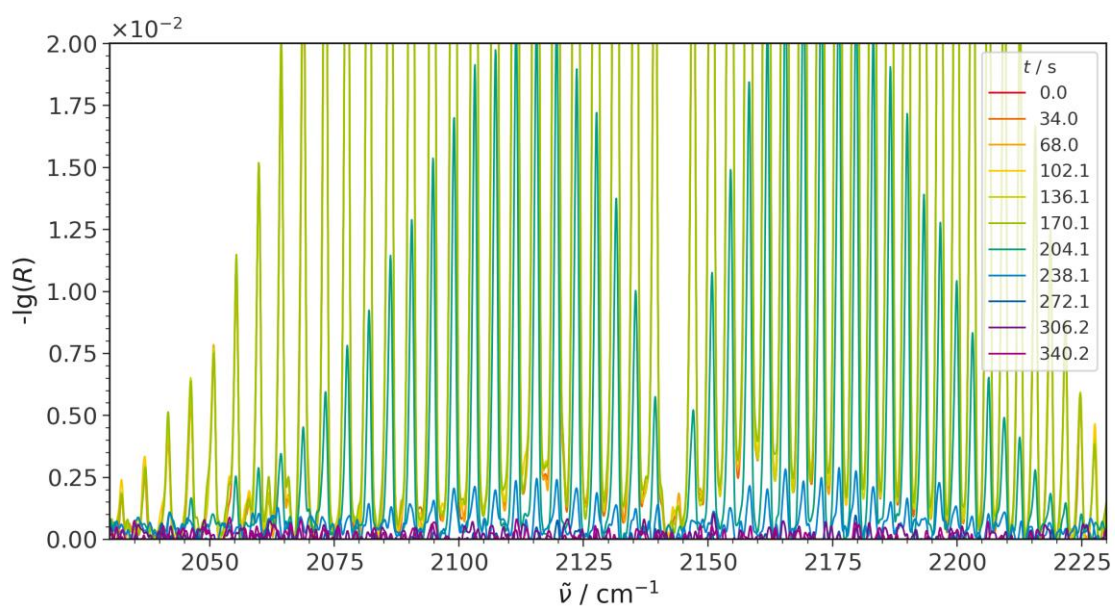
**Fig. S5: Top:** PSD spectra of the CO region of Au/CeO<sub>2</sub> (left) and CeO<sub>2</sub> (right) sheets after removal of gas-phase contributions. **Bottom:** Corresponding time shifts of individual spectral positions.

**Table S1:** Observed signals and their time values for gold-loaded ceria polyhedra. The same experiment has been executed three times and the maximum deviation  $\Delta_{\text{max}}$  for each signal is given in s.

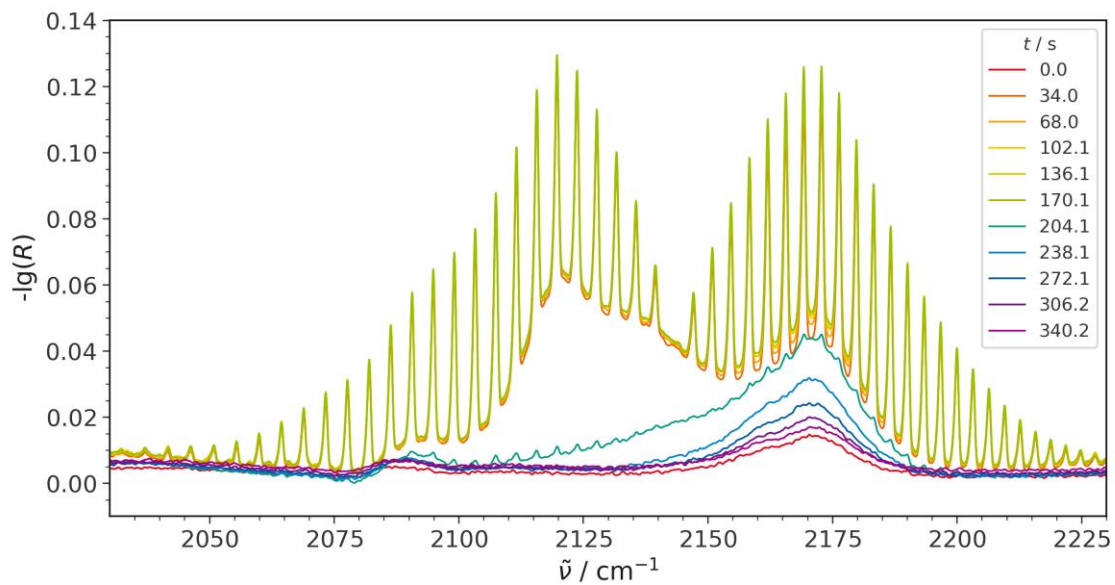
$\tilde{\nu} / \text{cm}^{-1}$	$t(\text{Au/CeO}_2 \text{ I}) / \text{s}$	$t(\text{Au/CeO}_2 \text{ II}) / \text{s}$	$t(\text{Au/CeO}_2 \text{ III}) / \text{s}$	$\Delta_{\text{max}} / \text{s}$
2092	18	21	21	3
2122	8	9	9	1
2133	9	11	11	2
2156	26	27	27	1
2171	42	43	42	1
2359	21	23	23	2



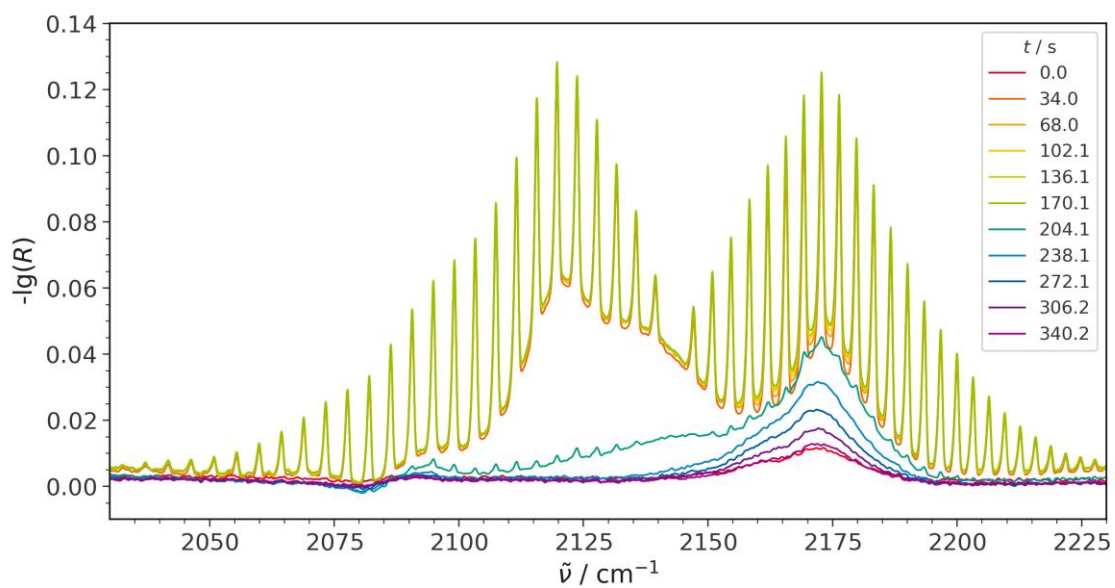
**Fig. S6:** Time-resolved spectra of the CO region of CeO<sub>2</sub> sheets.



**Fig. S7:** Time-resolved spectra of the CO region of Au/CeO<sub>2</sub> polyhedra.



**Fig. S8:** Time-resolved spectra of the CO region of Au/CeO<sub>2</sub> sheets.



**Fig. S9:** Time-resolved spectra of the CO region of Au/CeO<sub>2</sub> polyhedra.