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Experimental study of the Mechanism of High Temperature CO_2 Hydrogenation to Methanol over $ZnZrO_x$-based Catalysts

Aim

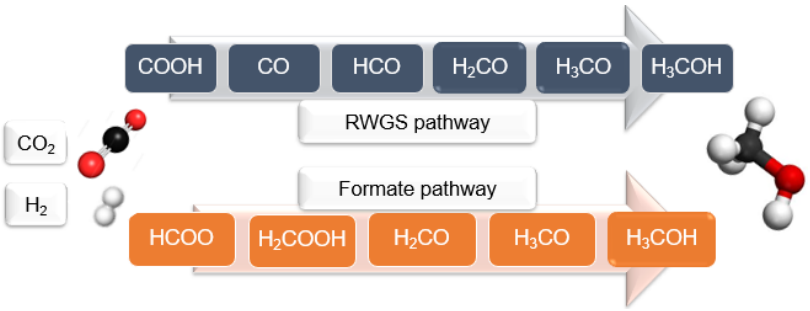
Elucidating the reaction mechanism, intermediates, spectators, and rate-determining steps in CO_2 hydrogenation to methanol synthesis at high reaction temperatures over $ZnZrO_x$-based catalysts using High-Pressure isotope-labelling experiments and DRIFTS measurements.

Justification

One way to mitigate CO_2 emissions is to convert it to valuable products, particularly methanol and light olefins, and close the carbon cycle. At the LCT, we developed a selective $ZnZrO_x$ catalyst, that can be used in a tandem process to produce light olefins via a methanol intermediate. While thermodynamically CO formation is favoured at the reaction temperature, a good catalyst selectively speeds up the formation of the less favoured product, methanol. Lack of a molecular view on the reaction mechanism hinders the design of even more selective catalysts.

Two main routes have been proposed in the literature (Figure). CO_2 is either hydrogenated first at the *carbon* atom, yielding formate and the reaction follows the formate route (H_2COO, H_2COOH, CH_2O, CH_3O), or CO_2 is hydrogenated first at the *oxygen* atom, yielding COOH and following the reverse water-gas shift pathway. Unfortunately, most of the proposed reaction intermediates cannot be detected in the gas phase, therefore their existence must be tested through other techniques.

The objective of this master thesis is to unravel the CO_2 hydrogenation mechanism over $ZnZrO_x$-based catalysts using an advanced *operando* DRIFTS cell to identify surface intermediate and spectators using their spectroscopic fingerprints. This study will be complemented by isotopic labelling kinetic experiments using our state-of-the-art high pressure SSITKA setup.



Program

1. Literature study: mechanistic studies of methanol synthesis over oxide catalysts.
2. Activity tests in the HP-PFR reactor.
3. *Operando* DRIFTS studies of CO_2 hydrogenation over $ZnZrO_x$-based catalysts to identify the reaction mechanism, surface intermediates, spectators, and rate-determining steps in methanol synthesis and in the CO-forming side reactions at high temperatures complemented by isotopic labelling kinetic experiments using SSITKA setup.

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