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ABSTRACT:

Dual Function Materials for CO_2 hydrogenation to methane: identification of active species through *Operando* techniques.

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The global warming associated to the increasing emissions of CO_2 in the atmosphere and the still current dependence on fossil fuels, at least in the mid-term, require the development of CO_2 capture and utilisation (CCU) technologies allowing conversion of CO_2 emissions from industrial processes into synthetic fuels and chemicals [1]. The effective integration of the CO_2 captured from flue gases and its subsequent methanation with renewable H_2 through a chemical looping process strongly depends on the development of highly performing Dual Function Materials (DFMs) containing both a sorbent and a catalytic component. This can avoid the energy intensive thermal swing process of adsorption and subsequent desorption of CO_2, followed by its catalytic hydrogenation [2].

The nature of the adsorbed species from the CO_2 capture step and their role in the subsequent hydrogenation step can be studied through *Operando* techniques such as TG-MS and *in-situ* DRIFT, simulating the conditions of the chemical looping process.

The selection of the best chemical DFM formulation and the proposal of a reaction mechanism, as well as the effect of other substances, such as O_2, H_2O and SO_2, typically present in the composition of real flue gases, are discussed focusing on the results of these techniques.

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[2] M. Abdallah, R. Farrauto, Catal. Today, 423, 113923 (2023).