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CO2 alcoholysis to organic carbonates over Zr-based catalysts: an in situ ATR-IR study

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Beside the reduction of CO₂ emissions by switching from fossil to renewable energy sources, alternative strategies to limit the greenhouse effect are represented by its storage and/or utilization. Among the various proposed utilization reactions, a potentially viable route is the direct CO₂ fixation in organic carbonates, whose industrial interest as green chemicals is growing [1].
This work focuses on the synthesis of simple organic carbonates through the direct reaction of CO₂ and alcohols: the main challenge is the high energy barrier of this reaction, which requires the development of effective catalysts to make it viable. We focus here on the development of specific heterogeneous catalysts, based on Zr⁴⁺ supported over high surface area silica, as inspired from the results on the corresponding pure oxide [2]. Furthermore, post-synthetic functionalization with amines is exploited to enhance the capture capabilities toward CO₂. A graphical concept of the catalyst is given in the attached Figure.
Beside the basic characterization outcomes, the first fundamental results on the interaction of the pure reactants (CO₂ and alcohols) with the proposed catalyst have been obtained by means of liquid phase in situ ATR-IR spectroscopy. The complex datasets have been treated also taking advantage of reference materials and is further corroborated by applying advanced analysis tools, such as concentration modulation experiments and multivariate curve reconstruction. Preliminary results concerning the reaction will be discussed too.
A valuable contribution to this project would result from the quantitative evaluation of the catalytic performances of the designed catalysts compared to ones of a reference, since only qualitative data are presently available.

[1] M. Aresta, A. Dibenedetto and A. Angelini, Chem. Rev., 2014, 114, 1709–1742.
[2] K. Tomishige, Y. Ikeda, T. Sakaihori, K. Fujimoto, J. Catal., 2000, 192, 355–362.

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