

Abstract 2CCO₂

'2 catalysts for CO₂' - Dual catalysis approach for the carboxylation of aliphatic olefins using CO₂ as the carbon source, full cSBO with a proposed starting date on 1 January 2022 and a proposed duration of 48 months, with partners KU Leuven, UAntwerpen and VUB.

This project aims at producing **chemicals that incorporate a high fraction** (≥ 50 weight %) of CO₂. The strategy is to reduce CO₂ to CO with H₂ and a solid catalyst at moderate temperatures (< 200°C), and to immediately consume the CO by coupling it in the same liquid phase reactor to other reactants, typically olefins like butadiene or ethylene. The equilibrium of the CO₂ reduction (a.k.a. the 'Reverse Water Gas Shift Reaction', RWGSR) is unfavourable at low temperature; we can circumvent this limitation by withdrawing the CO from the equilibrium and coupling it to an olefin in a homogeneously catalysed reaction. Comparing with other routes for CO₂ incorporation, our concept:

- (i) needs **only one H₂ per CO₂**, while e.g. CH₃OH production requires 3 H₂ per CO₂;
- (ii) works at much **lower temperature** (< 200 °C) than 'classical' CO₂ hydrogenation.

Success in this **high-risk approach** will depend on (i) design of shape-selective catalysts for the RWGSR (KU Leuven), (ii) use of innovative homogeneous catalysts that are efficient even at low CO pressures (UA), (iii) thorough insight of concentrations and traffic of CO₂, CO, olefins ... in the system (VUB).

This strategy offers new routes, with highly improved CO₂ footprint, to chemicals like for instance:

- **adipic acid** and its ester derivatives: adipic acid produced in this way will contain **60 mass% CO₂**;
- **acrylic acid**: coupling of CO₂ to ethylene (via CO) gives propanoic acid, which in a subsequent step can be dehydrogenated to acrylic acid, containing again **61 mass% of CO₂**.

Such a concept can be highly appealing for

- **producers of adipic acid, acrylic acid**, other carboxylic acids, looking for routes valorizing CO₂;
- producers of **polyamidefibers** (e.g. Nylon-6,6): they can get access to CO₂ based feedstock;
- producers of an array of **polyesters, polyols** (and **polyurethanes**) that are adipate based; etc.

For substantive questions about this project proposal, please contact MOT3 representative Luc Van Ginneken (lvanginneken@catalisti.be; +32 477 979 947).