

Supervisor(s) Prof. Mark Saeys	Period 4 years	Funding MuSE
--	--------------------------	------------------------

Development of low-temperature methanol synthesis catalysts.

Aim

The aim of this project is to develop catalysts for CO₂ hydrogenation to methanol under mild conditions.

Justification

Renewable energy imports originating from wind and sun will become a necessary and vital part of the EU energy mix. Currently, the most straightforward method of transporting renewable energy is liquid hydrogen. However, its low volumetric density and very low boiling point present major technical challenges. One of the strategies to avoid the transport of pure hydrogen is to produce hydrogen-derived green molecules. The derivatives of hydrogen, such as ammonia, methanol, and methane are considered green molecules when produced from renewable hydrogen and circular CO₂. Among these molecules, methanol (CH₃OH) has been pointed out as the most promising hydrogen carrier as it is liquid under atmospheric conditions, it owns one of the highest gravimetric and volumetric hydrogen storage capacities, and due to the existent widespread infrastructure for its transport.

Conventionally, MeOH is synthesized from syngas over heterogeneous catalysts, at elevated pressures (5-10 MPa) and moderate temperatures (220-300°C). However, MeOH can also be produced from other carbon-containing feedstock and its direct synthesis from CO₂ has been under the spotlight. The hydrogenation of CO₂ to MeOH is more challenging than that of CO due to the thermodynamic and kinetic stability of CO₂. With state-of-the-art catalysts, the one-pass methanol yield of the CO₂-based process is lower than that of the syngas-based process. MeOH synthesis is exothermic with a decrease in the number of molecules, meaning that high pressure and low temperature thermodynamically favor MeOH formation. Clearly, MeOH production would benefit from the development of improved catalysts active at lower temperatures.

In collaboration with CNRS Lille, the Saeys group has recently developed a new class of complex catalytic materials. These solid micellar catalysts (SOMIC) consist of a matrix, active sites incorporated in this matrix, and surfactants to stabilize the active sites (Figure 1). The first example of this family demonstrated unique performance in water-free CO₂ hydrogenation to formate in the presence of tertiary ethyl amine (TEA) and in the selective carbonyl hydrogenation in aqueous biomass-derived feedstock under mild conditions. We anticipate that low-temperature CO₂ hydrogenation over these heterogeneous catalysts can be directed towards methanol instead of formate.

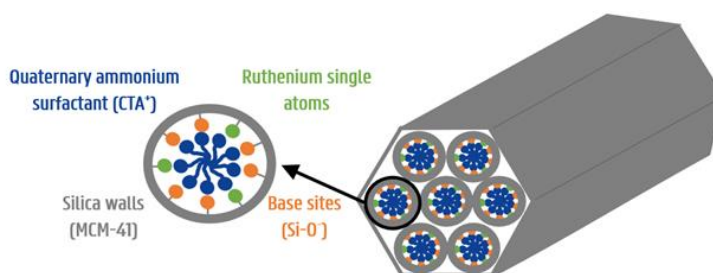


Figure 1. Schematic representation of the Ru^(III)@MCM-41 catalyst.

Program

- Catalysts synthesis and characterization;
- Evaluation of the performance of the catalysts in batch and continuous flow reactors;
- Optimization of reaction conditions.