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# Evaluating the performance of new solid micellar catalysts for $CO_2$ hydrogenation

## Aim

The aim of this project is to evaluate the performance of transition metal-based solid micellar catalysts (SOMIC) for the hydrogenation of $CO_2$ and its derivatives.

## Justification

Renewable energy imports originating from wind and sun will become a necessary and vital part of the EU energy mix. The most straightforward method of transporting renewable energy is liquid hydrogen. However, its low volumetric density and very low boiling point present technical challenges. One of the strategies to avoid the transport of pure hydrogen is to produce $H_2$-derived green molecules such as formate/formic acid, methyl formate and methanol via hydrogenation of $CO_2$ and its derivatives. Under this scenario, the development of cost-effective heterogeneous catalysts able to hydrogenate $CO_2$ to liquid hydrogen carriers is very important.

Solid micellar catalysts (SOMICs) are a new class of heterogeneous catalytic materials that contain isolated metal ion sites incorporated in the walls of a silica support and stabilized by surfactant molecules in the pores. The unique and well-defined coordination environment of the metal center in SOMIC looks like the one from homogeneous catalysts, in which the active sites consist of a transition metal atom or ion surrounded by ligands.

The first SOMIC catalyst synthesized, $Ru^{(III)}$@MCM (**Figure 1**), contains $Ru^{(III)}$ single-sites incorporated in the pore walls of MCM-41 stabilized by a cetyltrimethylammonium ($CTA^+$) surfactant. $Ru^{(III)}$@MCM is efficient and selective for the hydrogenation of carbonyl, double and triple bonds in aromatic compounds[1, 2]. Typically, the electronic structure of the metal, its oxidation state, coordination geometry, ability to undergo coordination changes during the catalytic cycle and its synergy with the surrounding atoms determine the catalyst activity, selectivity and stability.

Considering the conceptual and chemical similarity between our new $Ru^{(III)}$ single-site catalyst and the reported performance of first row transition metals-based homogeneous[3-5] catalysts, we believe that replacing $Ru^{(III)}$ by a more oxophilic metal ion like $Fe^{(III)}$, $Co^{(III)}$ or $Mn^{(III)}$ is a possible approach to simultaneously increase SOMIC stability and reduce catalyst cost.

While working on this project the student will have the opportunity to synthesize non-noble metal based-SOMIC materials and screen their performance under different reaction conditions.

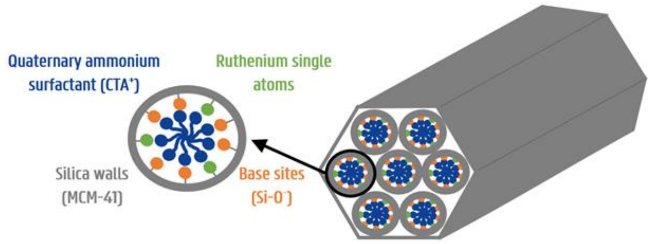


**Figure 1**. Schematic representation of the $Ru^{(III)}$@MCM-41 catalyst.[1]

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## Program

1. Literature study on transition metal-based homogeneous catalysts for low-temperature $CO_2$ hydrogenation.
2. Synthesis and characterization of new solid micellar catalysts.
3. Catalyst and reaction conditions screening using a batch setup.

## References

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