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A kinetic study on CO_2 hydrogenation to methanol

Aim

The aim of this project is to evaluate the performance and stability of a single-atom catalyst for low-temperature methanol synthesis based on the acquisition of kinetic data.

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 encountered 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 CO_2. Among these molecules, methanol (CH_3OH) 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)[1]. However, MeOH can also be produced from other carbon-containing feedstock and, in particular, its direct synthesis from CO_2 has been under the spotlight. However, the hydrogenation of CO_2 to CH_3OH is more challenging than that of CO due to the thermodynamic and kinetic stability of CO_2[2]. With state-of-the-art catalysts, the one-pass methanol yield of the CO_2-based process is lower than that of the syngas-based process[1]. 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.

Recently, we discovered a new single-atom catalyst[3, 4] with the potential to efficiently catalyze CO_2 hydrogenation to methanol under mild conditions. In this project, intrinsic kinetic data will be acquired using a Robinson Mahoney multiphase continuous flow reactor. The kinetic data collected during this project will allow us to identify which elementary steps control the reaction rate, how the rate is affected by reaction conditions and the catalyst's properties, and identify deactivation mechanisms — insights that are useful to guide the design of improved catalysts.

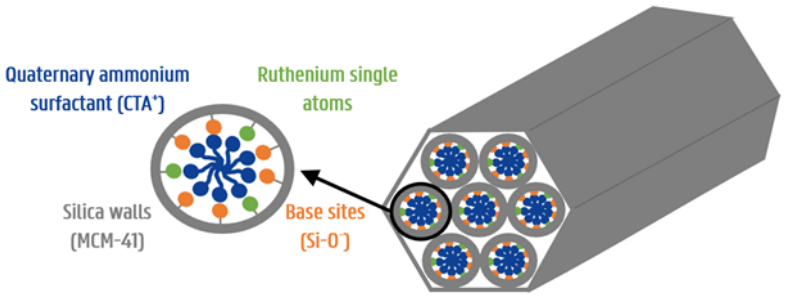

Figure 1. Schematic representation of the $Ru^{(III)}$@MCM-41 catalyst.[3]

Program

1. Literature study on the state-of-the-art catalysts for CO_2 hydrogenation to methanol.
2. Synthesis and characterization of a single-atom catalyst.
3. Lab-scale catalytic testing using a Robinson-Mahoney reactor.

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