

Coach	Supervisor(s)	Funding
Jan Oner Max Bols	Mark Saeys	MuSE

CO₂ Hydrogenation to Methanol: Your Chance To Reduce Your CO₂-Footprint!

Aim

Hydrogenation of carbon dioxide (CO₂) into methanol (MeOH) at low temperatures using single-atom catalysis in a high-pressure batch reactor.

Justification

The conversion of CO₂ to MeOH presents a dual opportunity to address climate change and enhance energy sustainability, making it a significant area of interest in chemical engineering. This process not only contributes to CO₂ recycling efforts but also produces methanol, a key chemical feedstock and potential renewable energy source. The relevance of this process is magnified within the context of chemical engineering education, where students can explore sustainable solutions to global challenges.

The hydrogenation of CO₂ to MeOH is thermodynamically favoured at low temperatures and high pressures due to its exothermic nature and reduction in entropy. Despite these favourable conditions, the industrial standard catalyst, Cu/ZnO/Al₂O₃, operates under relatively harsh conditions, requiring high temperatures that not only reduce the overall efficiency but also lead to only moderate yields of methanol. As shown in **Figure 1** these elevated temperatures facilitate the reverse water-gas shift reaction, a competing process that generates carbon monoxide (CO) and water, further complicating the direct synthesis of methanol and potentially degrading the catalyst through the oxidation of active sites and agglomeration of ZnO. These challenges underscore the urgent need for innovative catalyst designs that can operate effectively under milder conditions, thereby enhancing yield and selectivity towards methanol production.^[1,2]

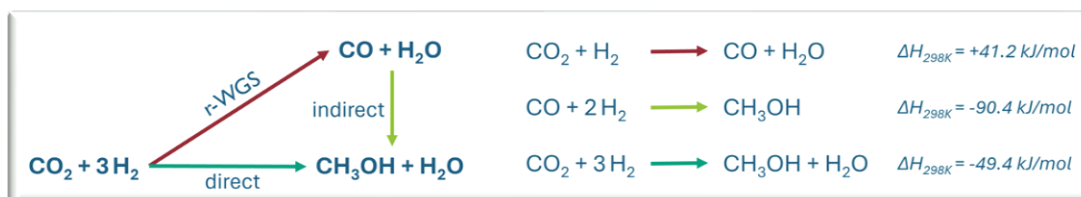


Figure 1: Possible reaction paths during the hydrogenation of CO₂. Thermodynamically, the exothermic nature of methanol synthesis favors the use of lower reaction temperatures.

Program

This project proposes to investigate a novel class of catalysts known as solid micellar catalysts (SOMIC), developed in collaboration with CNRS Lille. These catalysts leverage the principles of single-atom catalysis but introduce a unique mesoporous silica structure supporting isolated active Ru(III) sites. A distinctive feature of the Ru-SOMIC system, setting it apart from traditional single-atom catalysts, is the retention of the CTA⁺ micellar structure within its pores. This innovative design has demonstrated exceptional performance in the amine-assisted water-free hydrogenation of CO₂ to formate. Notably, removing the surfactant leads to a significant decrease in catalytic activity, underscoring the crucial role of CTA⁺ molecules in the catalyst's functionality.^[3–5]

The focus of this thesis will be on synthesizing and testing potential SOMIC catalysts within high-pressure batch reactors, with an aim to fine-tune the Ru-SOMIC system for enhanced selectivity towards methanol production. **Figure 2** outlines various strategies for modifying the Ru-SOMIC system to achieve this goal.

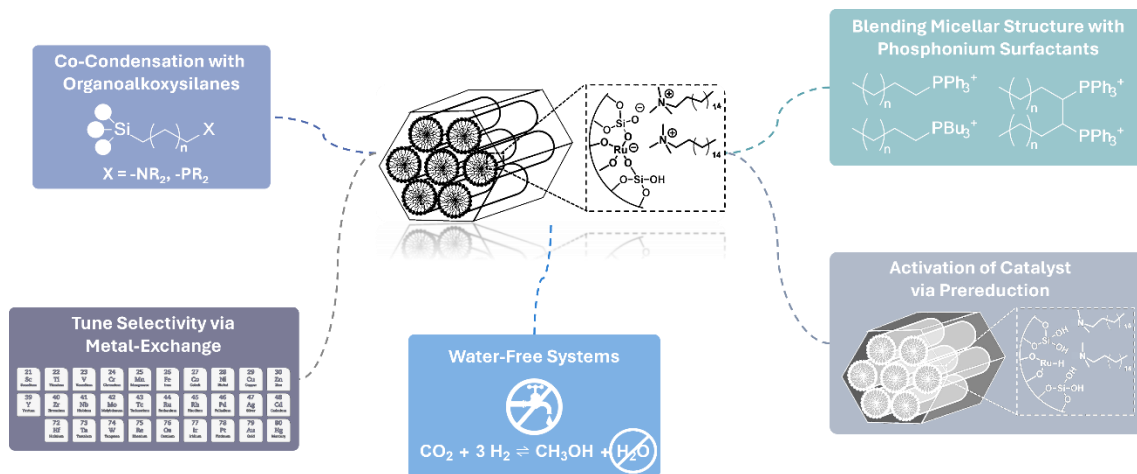


Figure 2: Potential strategies to tune the selectivity of the Ru-SOMIC system towards MeOH.

The research will employ diverse synthesis techniques alongside analytical methods such as high-performance liquid chromatography (HPLC), gas chromatography-mass spectrometry (GC-MS), nuclear magnetic resonance spectroscopy (NMR), and nitrogen physisorption analysis. These techniques will be central importance in characterizing the catalysts and monitoring reaction outcomes.

This project aims not only to advance the field of chemical engineering by introducing an innovative class of catalysts but also to offer chemical engineering students a valuable opportunity to engage with cutting-edge research.

References:

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