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Coach	**Supervisor(s)**	**Funding**
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Building realistic molecular models for CO_2 hydrogenation to formate

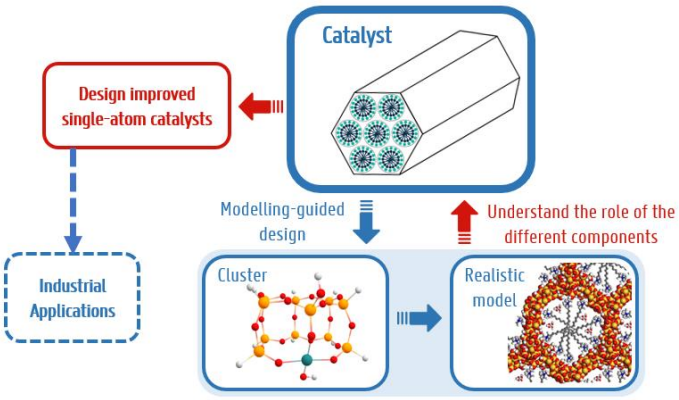
Aim

Modelling based insight in the nature of the activity and selectivity catalysts suitable for CO_2 hydrogenation to formate.

Justification

The hydrogenation of CO_2 to power molecules such as formic acid and methanol is receiving increased attention, due to both the environmental significance of greenhouse gas utilization and the industrial importance of fuel production. The conventional technology to produce formic acid is a multi-step process based on CO. The state-of-the-art in CO_2 hydrogenation to formic acid are homogeneous catalysts – virtually not stable and active heterogenous catalysts are known for this reaction. For this reason, we continue to work on the development of potential single-site heterogeneous catalysts for CO_2 hydrogenation. Our group is studying a particular catalyst that shows outstanding results for CO_2 hydrogenation to formate. A simple model was adopted to do the mechanistic studies using Gaussian 16. However, due to the complexity of the system a more realistic model is being developed (Figure 1).

Density Functional Theory (DFT) will be employed to guide the modelling of the active site and identify key factors that affect the catalyst activity (type of metals, reaction conditions, organometallic ligands). The mechanistic studies will be performed using Gaussian 16, while for the periodic calculations, VASP will be used.



Program

1. Literature study to investigate MCM-41 structures and modelling
2. Design and modelling of realistic models for single-site catalysts
3. Simulation of reaction pathways
4. Modelling-guided design