LABORATORY FOR CHEMICAL TECHNOLOGY
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Coach	**Supervisor(s)**	**Funding**
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Exploring the design space of Solid Micellar Catalysts for CO_2 hydrogenation

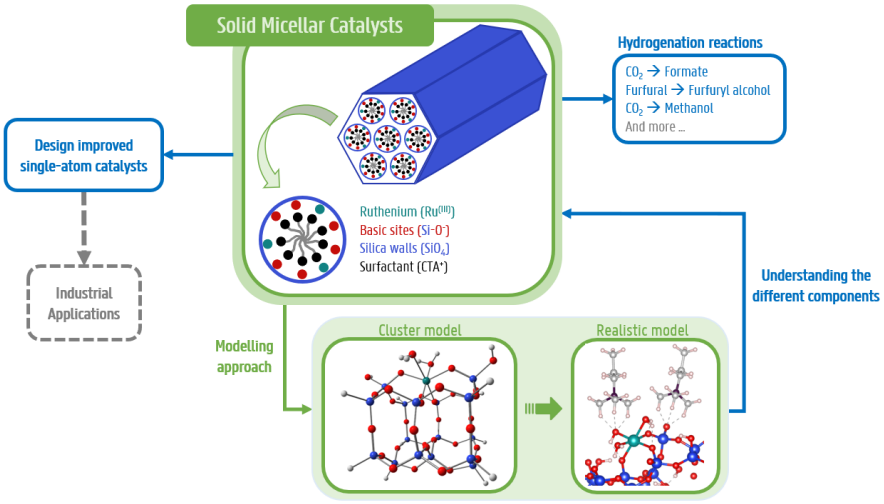
Aim

Modelling-guided studies of the nature of the active sites in Solid Micellar catalysts, to get insights on the components that affect the activity and selectivity for CO_2 hydrogenation to power molecules.

Justification

The potential of Solid Micellar catalysts as a platform to create newly active and selective catalysts for CO_2 hydrogenation to molecules such as methanol and formic acid is outstanding. This class of materials is composed of a single metal atom (e.g. $Ru^{(III)}$) incorporated into the walls of mesoporous silica (MCM-41) and stabilized by a quaternary ammonium surfactant. To fully understand the nature of the active sites and gather insights on the mechanism, a simplified cluster model was developed. However, a more realistic approach was also adopted, where we use a periodic structure model to explore H_2 activation, a key step in CO_2 hydrogenation reactions.

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, different surfactants, etc.). The mechanistic studies on cluster models will be performed using Gaussian 16, while for the periodic calculations, Vienna Ab Initio Simulation Package (VASP) will be used.



Program

- Literature study on modelling of mesoporous silica and surfactant-filled pore structures.
- Design and simulation of realistic models for single-site catalysts.
- Simulation of reaction pathways.
- Modelling-guided design of novel solid micellar catalysts.

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