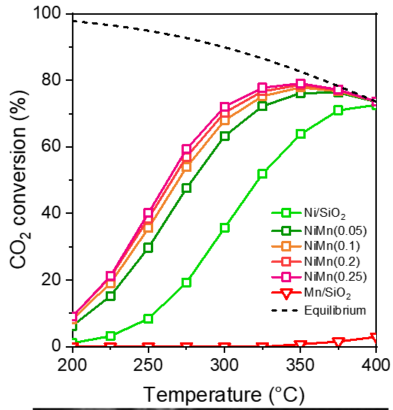
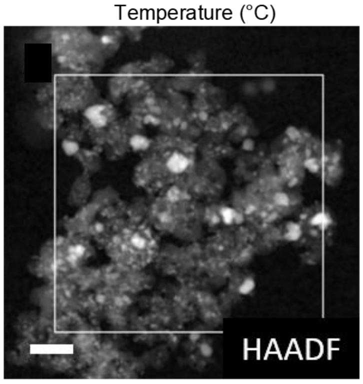
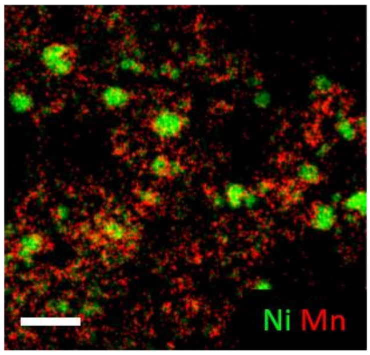
Inorganic Materials & Catalysis
Molecular Heterogeneous Catalysis
Research Project – Emiel Hensen/Jérôme Simons

CO_2 from waste to resource: Unraveling the effect of metal-metal oxide cluster interactions in catalysts for the Sabatier reaction

Identified as a potential energy and water source for long-term manned missions to Mars by NASA, the Sabatier reaction has received much attention recently for the conversion of waste CO_2 [1]. In this reaction CO_2 reacts with renewable H_2 (e.g. from water electrolysis) to form CH_4 and H_2O. The produced methane can be injected directly into the existing natural gas infrastructure and therefore this reaction is targeted as a way to convert green electrical energy into high value chemical energy carriers. Current technology however does not offer sufficiently active and cheap (scalable) catalysts for promoting this reaction.







Conceptually, we have shown that the combination of Ni with MnO clusters yields a very high activity in CO_2 reduction to CO [2]. A combination of kinetic and spectroscopic investigations showed that a direct pathway competes with a carbonate pathway at the surface. Density functional theory demonstrated that the direct pathway provides much lower barriers and follows a mechanism in which oxygen defects are created in MnO, which opens a pathway of low-barrier CO_2 and CO dissociation.

As a next step, we wish to explore the wider utility of this concept by exploring alternative combinations of metal and metal oxides. These catalysts will be extensively characterized for their performance in CO_2 hydrogenation. A high-throughput setup will be available for rapid screening of the performance of catalysts. A high-pressure setup will be used to evaluate the performance of CO_2 hydrogenation at conditions deemed optimal for synthetic natural gas production. These catalysts will be characterized in more detail by XRD, XPS, Chemisorption, TPR, TEM and FTIR.

Within this project, you will be searching for an optimum catalyst for the conversion of CO_2 to methane by investigating the effect of metal-metal oxide cluster interactions. Here different catalyst preparation methods, supports (e.g. TiO_2, SiO_2, Ce-ZrO_2) and active metals (Ni, Co) will be used.

Learning goals:
- Become familiar with catalyst preparation and characterization methods that are highly relevant in both industry and academia.
- Construct relevant research questions and a working hypothesis.
- Build a research report based on the research topic and present the results in an oral contribution.

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[1] C. Vogt et al., *Nat. Catal.*, 2019, **2**, 188-197
[2] W. Vrijburg, *PhD Thesis*, 2019