FACULTY OF **ENGINEERING AND ARCHITECTURE**

Department of **Chemical Engineering and Technical Chemistry**
Laboratory for Chemical Technology
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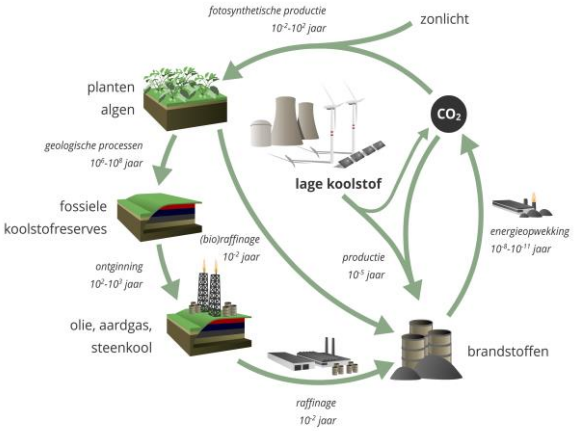
Modeling guided design of selective catalysts for catalytic CO_2 reduction

Aim

Develop catalytic processes to activate CO_2 and introduce CO_2 as an extension block to add value to base chemicals.

Justification



Closing the carbon cycle through catalysis.

The necessary transition to ***CO_2-neutral*** human activity introduces immense scientific and technological challenges. Our high standard of living relies heavily on carbon-based materials and high-density energy carriers. A drastic move away from a carbon-based society is not expected. The accumulation of CO_2 in the atmosphere is a ***timing problem*** – CO_2 is produced at a much faster rate than natural processes consume it. In this project we develop catalytic materials to re-activate CO_2 with a productivity (kg $CO_2/m^3_{reactor}$ s) and an efficiency commensurate with the tremen-dous rate of CO_2 production in order to close the carbon cycle. Such a productivity can only be achieved by catalytic processes. The reductive power to activate CO_2 will be supplied by H_2 produced from low-CO_2 energy sources such as solar energy. Catalyst design and kinetic modeling often start from molecular-scale hypotheses about the reaction mechanism, the structure of the active catalyst and the nature of the rate and selectivity determining steps. Computational catalysis has become a crucial tool to analyze molecular-scale concepts and elucidate their electronic origin. In combination with characterization and experimental kinetic validation, insights gained from computational catalysis can be translated all the way to the industrial scale. This pas-de-deux between experiment and theory is becoming the new paradigm in catalyst design and kinetic modeling, both in academia and in industry.

References
Banerjee, van Bavel, Kuipers, Saeys, ACS catal. **2015**
Zhuo, Borgna, Saeys, *J. Catal.* 297, 217, **2013**
Tan, Chang, Borgna, Saeys, *J. Catal*., 280, 50, **2011**

Program

The project extends our experimental and modeling experience with CO hydrogenation (Fischer Tropsch synthesis) to CO_2 hydrogenation. We will start by studying the hydrogenation of CO_2 to methane and methanol, but expect to expand the scope by studying reactions related to hydroformylation and carboxylation which use CO2 as an extension unit to add value to base chemicals.

Advisor: Prof. Dr. ir. Mark Saeys

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