CO_2 Hydrogenation

CO_2 capturing and utilization technologies have the potential of decreasing the CO_2 emissions that cause climate change. Utilization of CO_2 also allows to directly recycle the CO_2 produced in the industry to make the process carbon neutral and to produce value-added products (fuels and chemicals). Methanol is an excellent product for CO_2 utilization, since it is already produced world-wide in large scales to be used as a fuel and a solvent.

CO_2 hydrogenation is an excellent candidate technology to convert captured, or recycled CO_2 into methanol. This technology is currently used in the industry to convert a CO rich mixture of $CO_2/CO/H_2$ into methanol. The most important component of this technology is the catalyst, which has already been optimized for the specific CO rich $CO_2/CO/H_2$ mixtures available in industrial processes. For captured or recycled CO_2 utilization, more CO_2 is expected in the feedstock mixture and a new catalyst optimization needs to be carried out.

Challenges

One of the main challenges in catalyst research is catalyst deactivation, which is more prominent when more CO_2 is present in the feedstock mixture. CO_2 catalysts for CO_2 hydrogenation are complex nanostructures with at least 2 elements mixed in the nanoscale. In order to study and optimize catalysts for CO_2 utilization, catalytic properties of complex alloyed catalysts need to be screened efficiently.

TECHNICAL INPUT

Particle Source	VSP-G1 & VSP-S1
Deposition Method	Diffusion
Deposition System	S1
Deposition Parameters	N/A
Sample	SiO_2 support for fix bed reactors
Material	Transition metals
Application	CO_2 Hydrogenation
Analysis technique	TEM

Solution

The nanoparticle generator (VSP-G1) of VSPARTICLE can produce a nanoscale mixture of transition metals and alloys of virtually any composition. This opens up the possibility to optimize the screening for composition-dependent catalytic properties. The operation of the G1 is at ambient temperature and pressures, which allows a quick exchange of target materials. Some of the complex catalytically active sites that can be engineered with VSPARTICLE tools are illustrated below.

Example experiment setup

Set-up for alloy nanoparticles decorated with single size oxide particles.

In this example set-up, alloyed nanoparticles are produced by the VSP-G1, while single size oxide particles (e.g., In_2O_3) are produced in the VSP-S1. The alloyed and the single size oxide particles are then mixed directly in the gas phase and deposited by diffusion. With this set-up any of the complex active sites illustrated below can be obtained and optimized by tuning the size and composition of each nanoscale component.

Engineering complex active sites with VSPARTICLE tools