LABORATORY FOR CHEMICAL TECHNOLOGY
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Supervisor(s)	**Period**	**Funding**
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Atomic scale design of CO_2 conversion catalysts

Aim

In the project, you willemploy an atomistic approach to selectivity and stability in heterogeneous catalysis by studying structural and kinetic properties and chemical reactivity of nano-engineered model catalysts for CO_2 conversion reactions, prepared by ALD with full site control.

Justification

Today's challenge for the chemical industry is ensuring sustainable supplies of fuels, chemicals and materials for a growing global population, while limiting global warming and climate change[1]. Controlling the atmospheric CO_2 level forms an inseparable part of this evolution. Catalytic technologies will play a pivotal role in addressing this challenge throughout the 21st century by enabling the utilization of alternative energy sources and feedstocks, mitigation of greenhouse gases, and pollution abatement. At the heart of these processes are efficient catalysts, which not only need to be **active**, but also highly **selective**, ideally reaching 100% selectivity, and **stable**.

CO_2 conversion catalysts - CO_2 can be hydrogenated to hydrocarbons either directly or indirectly, e.g. via syngas. Direct conversion includes the production of urea, salicylic acid, dimethyl carbonate, polyurethane, polycarbonate, polyacrylates and (in)organic carbonates. Further, CO_2 can also be hydrogenated into chemicals or fuels such as methane, formaldehyde, dimethyl ether, formic acid, methanol and other alcohols. Additional options lie in its use as mild oxidant, e.g. in CO_2-assisted dehydrogenation of alkanes to form alkenes, water and CO. The activation of CO_2 and its hydrogenation to hydrocarbons or alcohols are challenging because CO_2 is very stable, requesting co-reagents and efficient catalysts.

Program

- Stabilized Rh and Pt NPs with inert Al_2O_3 and SiO_2 coatings will be used. The accessibility of the catalyst surface after coating will be investigated by CO adsorption and the impact on sintering/stability will be evaluated by in situ X-ray scattering experiments during calcination
- Edge/facet-selective ALD coating of Pt and Rh NPs with inert (MgO) and redox-active (Co- and Fe-oxide) coatings will be used. The coating morphology will be evaluated by CO-adsorption, and the impact on activity and selectivity for CO_2 methanation and ethanol synthesis reactions will be assessed.
- ALD coating of redox-active Ni NPs with inert (MgO) and redox-active (Co- and Fe-oxide) coatings will be explored. Redox cycling will be applied to study redox behavior/alloying. The impact of the coating type on selectivity and stability (coke formation) for CO_2 dry reforming reactions will be assessed.

	Methods
Material characterization	XRD, TPR-TPO-TPD, ICP, TEM, XAS
Kinetic characterization	Operando XAS, TAP
Stability	Plug flow reactor
Selectivity	TAP, plug flow reactor

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