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Development and characterization of novel catalysts for methanol synthesis from CO₂ and hydrogen

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Catalysis will play a crucial role in all technologies, which potentially could be used for producing sustainable chemical fuels from solar energy. DTU CASE (Catalysis for Sustainable energy) has the main objective to overcome some of the catalyst challenges within this field by developing a science-based rational design strategy for new catalysts and to establish an understanding of the mechanism by which solid surfaces act as catalysts for energy conversion processes.

One specific challenge concerns energy conversion based upon decentralized hydrogen production. One solution could be to store hydrogen on location by methanol synthesis under lower pressure conditions. In the search of catalysts that might open up new processes, studies based on density functional theory (DFT) calculations have predicted a nickel gallium alloy to be active for this reaction [1].

NiGa catalysts prepared by incipient wetness impregnation on a high surface area silica support, have shown comparable turn over frequencies as the preferred commercial Cu/Zn/Al₂O₃ catalyst system [2]. This illustrates nicely that the DFT-predicted catalyst actually works for methanol synthesis and thereby that the rational design strategy has succeeded.

The catalysts have been studied and characterized extensively by activity measurements, in situ XRD and Environmental Transmission Electron Microscope (ETEM) [3] during nanoparticle formation, methanol synthesis, and accelerated aging experiments [2]. For the optimal Ni:Ga ratio of 5:3 in situ XRD and ETEM studies confirms the formation of the δ -Ni₅Ga₃ phase nanoparticles at temperatures above T>600°C in H₂. During methanol formation in 25% CO₂ in H₂ a significant deactivation is observed at temperatures 210°C<T<250°C. A regeneration of the catalyst can be obtained by a heat treatment at 300°C in pure H₂. At higher temperatures 300°C<T<400°C the catalyst is deactivated further, and a phase change from Ni₅Ga₃ to the less active Ni₃Ga is observed. In order to regenerate the catalyst a heat treatment at 700°C in pure H₂ is necessary [3].

The science-based rational design strategy will be the framework for further investigations on the promising NiGa catalyst for methanol synthesis in order to increase the long term stability of catalytic activity.

References:

- [1] F. Studt et al., SLAC, Stanford University (to be published).
- [2] I. Sharafutdinov et al., Technical University of Denmark (to be published).
- [3] T.W. Hansen et al., *Materials Science and Technology* 11(2010), p. 1338.