MS18-05 | Structural Insights into Methanation Catalysts from MOF-Precursors via PDF

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The conversion of CO_2 to methane using H_2 from water electrolysis is a promising approach to tackle the challenge of long-term energy storage based on energy from renewable resources. Because of fluctuations in the H_2 supply due to dynamic changes in wind and solar energy, a highly stable catalyst, which resists H_2 dropouts, is needed for the methanation reaction. Supported Ni nanoparticles are typical catalysts, yet prone to deactivation by surface oxidation or sintering under fluctuating conditions [1]. Catalysts derived from metal-organic framework (MOF) precursors via thermal decomposition are promising materials due to the fine dispersion of active centres [2]. We have synthesized Ni(BDC)(PNO) MOFs (BDC=benzene-1,4-dicarboxylate, PNO=pyridine-N-oxide), which were thermally converted into stable methanation catalysts consisting of Ni clusters or nanoparticles on a carbonaceous, amorphous support. With pair distribution function (PDF) analysis of total scattering data we target the structural transitions from the crystalline MOF to the nanostructured catalyst, since the PDF is a histogram of interatomic distances and, in contrast to traditional crystallographic approaches, does not require crystallinity within the sample to refine its structure. Both lab and synchrotron PDF data show that the structure of the Ni nanoparticles as well as of the carbonaceous support depend on temperature and atmosphere (reducing, inert) of the thermal decomposition. Structural insight into these mechanistic steps of catalyst formation will allow a future targeted design of catalysts from MOF precursors.

[1] B. Mutz et al., *Catalysts* **2017**, *7*, 279
[2] R. Lippi et al., *J. Mater. Chem. A* **2017**, *5*, 12990