Session of Focus Materialchemie – Wednesday, **07.12.2022** 16:00 – @ Seminarraum Lehar 02 (TU-Wien, Getreidemarkt 9, BC, OG. 02, room A46) – join us on ZOOM (ID: 983 0066 2349)

Perovskite Oxides for the Reverse Water-Gas Shift Reaction – Increasing Catalytic Performance by Nanoparticle Exsolution

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Perovskite Oxides (general composition ABO_3) with reducible transition metals on the B-site have been shown to exsolve these transition metals upon selective reduction, forming nanoparticles on the surface. This results in smartly designed catalysts, with a perovskite backbone decorated by well distributed, catalytically active particles. Compared to other methods, the preparation is simple and efficient and the active catalyst surface shows increased stability towards degradation (e.g. sintering or carbon deposition).

In the scope of the here presented thesis, such materials have been applied for the reverse water-gas shift reaction (rWGS), which takes CO_2 and H_2 to produce CO and H_2O. Thus, rWGS can be used as an important step in CO_2-utilisation, as the resulting CO can be, with addition of further H_2, transformed to various valuable products such as hydrocarbons (via Fischer-Tropsch reaction) or methanol. Perovskite oxides with exsolved nanoparticles are very well suited for this reaction due to their ability of job-sharing: while the oxygen defect perovkskite support is beneficial for CO_2-activation, the metallic nanoparticles enhance activation of H_2. Furthermore, their high stability is necessary for the required high temperatures.

The focus has been placed on two different approaches to optimise the catalytic performance. First, the composition of the materials has been varied, with the perovskite $Nd_{0.6}Ca_{0.4}FeO_{3-\delta}$ as a starting point. This included changing the A-site elements and their ratio, as well as introducing various dopant elements (Co, Ni, Cu) on the B-site. Second, the conditions for exsolution and rWGS operation, such as temperature and gas composition, have been investigated, in order to find out the relation between parameters of the exsolution process, the resulting particle properties and hence the catalytic behaviour under different rWGS conditions. A number of methods have been employed for characterisation, for example XRD, XPS, SEM, and catalytic testing, including operando techniques and synchrotron studies. In this talk, some exemplary results will be presented.

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