Doped Perovskite Oxides as Versatile Catalysts

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Abstract
A very versatile class of catalyst materials that can be used for applications in (electro)chemical energy conversion are perovskite oxides. They have the general formula ABO_3 and the high flexibility is due to the fact that the properties can be tuned by the choice of the cations A and B. These represent different sites in the crystal structure, and either site can be occupied even by a combination of elements. This allows adapting a material to the specific catalytic problem, e.g. by doping with a catalytically highly active element. Furthermore, the stability can be tuned and thermally stable materials are achievable, suitable for high temperature applications.

One of the reasons why perovskites excel in catalytic applications is their ability to exsolve metal nanoparticles consisting of the catalytically active doping elements, which consequently decorate the material surface. These nanoparticles are very stable towards sintering and coking, because they well socketed within the perovskite support.

The catalytic ability of perovskite oxides has been demonstrated for the reverse water-gas shift reaction (rWGS), transforming CO_2 and H_2 to CO and H_2O. This is an important reaction for energy conversion related processes. For example, CO could subsequently be used to produce fuels via Fischer-Tropsch synthesis. An element known to be beneficial for catalysis of rWGS is Cobalt, thus the Co-doped perovskite $Nd_{0.6}Ca_{0.4}Fe_{0.9}Co_{0.1}O_{3-\delta}$ (NCF-Co) was investigated. During reaction, the material showed exsolution of Co-nanoparticles, enhancing catalytic activity (Fig. 1). Characterization of the catalyst was performed with several methods, including *in situ* x-ray diffraction (XRD), *in situ* x-ray photoelectron spectroscopy (XPS) and scanning electron microscopy (SEM).

The concept could be extended to other reaction systems as well, such as methane dry reforming or methanol synthesis, using a suitable dopant element for the respective reaction. In addition, the composition of the perovskite (e.g. A-site elements) can be further tuned to the desired application, e.g. for temperature stability or lower costs.

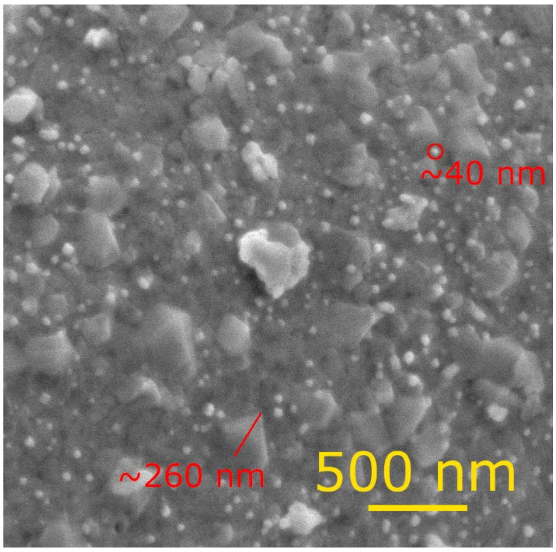

Figure 1: SEM image of NCF-Co after rWGS.

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