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New materials for hydrogen storage

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Hydrogen is recognized as a potential and extremely interesting energy carrier system, which can facilitate efficient utilization of unevenly distributed renewable energy. Here we report an overview of our recent results within (***i***) structural characterization of novel metal borohydrides, (***ii***) detailed studies of reaction mechanism during formation, and hydrogen release and uptake, and (***iii***) different experimental approaches for *in situ* powder X-ray diffraction at variable temperature and pressure for studies of gas-solid reactions [1,2].

A fascinating structural chemistry is discovered within metal borohydrides, *e.g.* 'MOF-like' networks with up to 30 % 'empty' space in the porous structures with chemical bonding ranging from ionic to more covalent and containing composite polynuclear complex anions in the solid state. Magnesium borohydrides form the most open-structured material (ρ = 0.55 g/cm^3), capable of physisorption of molecular hydrogen, *i.e.* γ–$Mg(BH_4)_2{\cdot}0.80H_2$, ρ_m = 17.4 wt% H_2 [3]. We also demonstrated that systematic mechano-chemistry (ball-milling) combined with *in situ* powder X-ray diffraction is a very efficient method for exploring new materials as demonstrated recently with the discovery of several cadmium based borohydrides [4]. A wide range of new materials is presented along with trends in structures and properties extracted from PXD data. In this talk, we will also illustrate that *in situ* powder X-ray diffraction is a unique, sensitive and informative technique for probing gas-solid reactions [1,2,6]. A new sample holder is tested at PETRA III, which can be operated at pressures up to 700 bar.

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