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Neutron Diffraction Investigations on Sorption Processes of Metal Organic Frameworks

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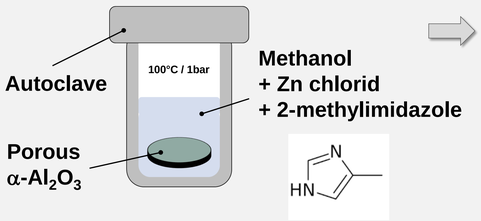
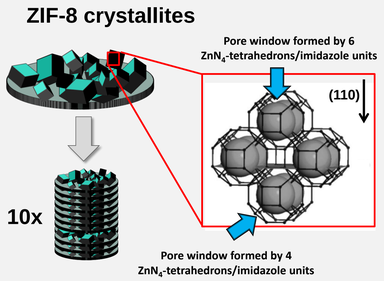
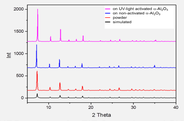
Metal Organic Frameworks ZIF-8 on α-Al_2O_3 membranes

Metal Organic Frameworks (MOFs) are considered as a new material class and have been studied intensively in the last decade. MOF represent, due to their huge nanostructured pore systems and manifold material properties a promising potential for research and innovation, affecting various technology sectors. This holds in particular true for systems, in which gas-solid interactions are of relevance (e.g. sensor technology). As neutron diffraction provides the only method to study structural changes in the interior in lager volume fractions of such materials, it appears as a suitable in-situ method to observe the impact of gas sorption on such substrates. For this purpose, the strain diffractometer EPSILON at IBR-2 is a promising tool to perform cutting-edge investigations. In this regard, a special experimental setup was developed. Recently, first experimental results have been taken and are shown in this contribution.

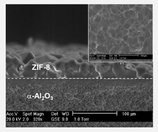
Solvothermal deposition







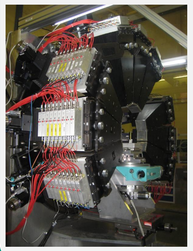
XRD patterns for ZIF-8 powder and SURMOFs deposited by the solvothermal method.

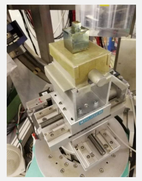


Electron microscope cross section and top-view (inset) image of a ZIF-8 coated macro-porous alumina membrane.

Experimental

The neutron time-of-flight strain diffractometer EPSILON: The multi-detector system allows to detect nine different directions at 2Θ = 90°, each of the nine detector banks is equipped with nine detectors to cover a wide range of solid angle. The instrument has been used as a powder diffractometer by summarizing the diffraction pattern of all 81 detectors.



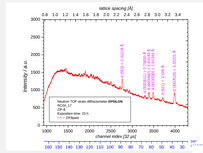


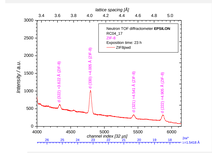
ZIF-8/Al_2O_3 pellets in vanadium container on the goniometer table.

Samples used in experiments (from left to right): ZIF-8 powder, ZIF-8 covered Al_2O_3 pellets, ZIF-8/Al_2O_3 pellets during washing in D_2O.

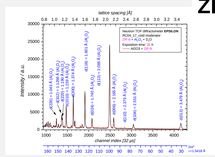
Neutron TOF diffraction

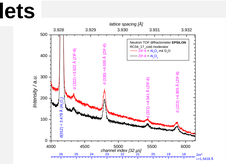
ZIF-8 powder





ZIF-8/Al_2O_3 pellets





The detected diffraction pattern cover a range up to λ_{max}= 7.1 Å (d_{max}= 5.1 Å), so that the metal organic framework samples could be characterized relating its properties.

Concluding remarks and outlook

- The results of the tentative investigation by the EPSILON instrument indicate, that the structural properties MOFs can be investigated with a high precision. In particular, first comparative study of ZIF-8 before and after exposure to D_2O, respectively, clearly shows an increase of the inelastic background.
- These results represent a promising base for the planned further investigation of *in situ* gas/solid interaction of MOFs with an use of a special gas system, which is under construction now.