



Contribution ID: 127

Type: **Poster**

Pore filling mechanism in the chemically stable Metal-Organic Framework DUT-67(Zr) by Neutron Powder Diffraction

Monday, 17 September 2018 17:45 (15 minutes)

Metal-Organic Frameworks (MOFs) –hybrid inorganic-organic porous crystalline materials with large and tunable pore structure, surface area and pore volume. The hierarchical pore structure of MOFs and tunable polarity of the inner surface make this class of materials attractive for the application in adsorptive heat pumps. Recently, a chemically stable microporous Zr-based MOF with composition $\text{Zr}_6\text{O}_4(\text{OH})_4(\text{tdc})_4(\text{CH}_3\text{COO})_4$ (tdc –2,5-thiophenedicarboxylate) and hierarchical pore structure was synthesized in our group. It possesses a BET area of $1250 \text{ m}^2\text{g}^{-1}$, total pore volume of $0.5 \text{ cm}^3\text{g}^{-1}$ and shows outstanding stability against water. The material shows desired for the adsorptive heat pump application S-shape water adsorption isotherm and therefore is potentially suitable for adsorptive heat storage applications. In order to shed a light on the mechanism of the water adsorption activated and D_2O -pre-loaded materials were subjected to the neutron powder diffraction (NPD) study at SPODI instrument of FRM II. Rietveld refinement of the NPD patterns show that the first water molecules are adsorbed at the preferable adsorption sites near the $\mu_3\text{-O}$ atoms of Zr_6O_8 cluster and trigonal window of the octahedral pore. Further the pore filling proceeds by filling smallest octahedral pore over a middle cuboctahedral and large cuboctahedral pores.

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Session Classification: Poster session 1

Track Classification: P8 Functional materials and materials science