Exploring water harvesting potential in CAU-10-H: an in-situ high resolution powder diffraction study

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Several metal-organic frameworks (MOFs) excel in harvesting water from the air or as heat pumps as they show a steep increase water uptake at 10-30 RH% [1]. Yet, a precise understanding of which structural characteristics leads to such behaviour is lacking [2]. We studied CAU-10-H and unravelled the materials’ structural deformation and water ordering during adsorption with in situ X-ray diffraction (see Figs. 1 & 2). In CAU-10-H, an energetically favourable polar water cluster is formed in the hydrophobic cavity, tethered via H-bonds to the framework m-OH groups. We conclude that favourable water adsorption occurs when sites of intermediate hydrophilicity (e.g. M-OH’s) are present in an otherwise hydrophobic structure, and the geometry and positioning of sites capable of hydrogen bonding allow the formation of an energetically favourable water cluster [3].

Figure 1. In-situ relative humidity experiment demonstrating the effect of temperature on the phase transition in CAU-10.

Figure 2. a) Expanded CAU-10-H cavity with water cluster, b) Rietveld refinement of the powder diffraction data for CAU-10-H.