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Keywords: metal-organic framework; crystal engineering; X-ray powder diffraction

FA4-MS08-P08

Structure Influence on Sorption Properties in a Dynamic Metal-Organic Framework Based on Calcium. Víctor A. de la Peña-O'Shea^a, Ana E. Platero-Prats^b, Natalia Snejko^b, Ángeles Monge^b, Enrique Gutiérrez-Puebla^b. ^aInstituto Madrileño de Estudios Avanzados en Energía (IMDEA Energía). ^bInstituto de Ciencia de Materiales de Madrid (ICMM-CSIC). E-mail: victor.delapenya@imdea.org

The design of new porous 3D polymeric structures is becoming increasingly important, due to their applications as catalysts and molecular sieves. Over the last years, metal-organic frameworks (MOFs) have emerged as an important new class of nanoporous materials with potential applications as gas storage and separation, catalysis, and chemical sensing. Nowadays, there is growing interest in metal-organic frameworks (MOFs) with flexible and dynamic frameworks, in particular, those that reversibly change their structures and properties in response to external stimuli as they may be used as sensors [1]. However, porous materials which have both high framework stability and framework flexibility are rare [2].

To date, MOFs have been proved to be promising materials for gases adsorption and separation (e. g. H_2 , CH_4 , CO_2 [3]. Moreover, recently the use of a flexible MOF for hydrocarbon adsorption in vapor phase was reported [4]. Understand the influence of flexibility on liquids sorption in MOFs would be of great interest in order to determine to what extent liquid adsorption can lead reversible structural changes.

Herein, we report a novel MOF based on calcium which shows an unusual guest-dependent dynamic behavior. This study relates the sorption of both liquids and vapors of different common solvents and gases in terms of adsorption capability and sorbate/sorbent interactions which cause reversible phase transition. In particular, the connection between structure changes and guest molecules was carefully investigated.

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Keywords: organic inorganic hybrid materials; adsorption; structural properties

FA4-MS08-P09

Controlled Growth of Metal-Organic Frameworks (MOFs) on Functionalized Organic Surfaces. <u>F.</u> <u>Wieland</u>^a, O. Shekhah^b, M. Paulus^a, C. Sterneman^a, M. Tolan^a, C. Wöll^b. ^aFakultät Physik/DELTA, Technische Universität Dortmund, Germany. ^bPhysikalische Chemie, Ruhr-Universität Bochum, Germany. E-mail: florian.wieland@uni-dortmund.de

Metal-organic frameworks (MOFs) are a new class of advanced materials which may be used for various applications. In contrast to the usual synthesis protocol a new approach for the synthesis of MOFs was developed in order to investigate the dynamics and the process of the structural formation [1]. Thin films of the MOF [Cu₂BTC₂(H₂O)] (HKUST-1) are grown by layer-by-layer deposition on top of functionalized organic surfaces which serve as a two dimensional nucleation site [2]. The samples were investigated by x-ray diffraction at the beamline BL9 [3] of the synchrotron light source DELTA. Two dimensional scattering patterns were obtained giving information about the structural order of the films. Comparing x-ray diffraction data of the corresponding bulk material with our data we find that layers of HKUST-1 grow in different preferred directions depending on the functional group of the self assembled monolayer. Also the structural behavior under temperature load was investigated up to a temperature of 320°C. The data shows that the network maintains its structure up to 300°C.

By replacing the the organic ligand by bezendicarboxylicacid a new MOF can be fabricated. X-ray diffraction patterns show that this MOF exhibits a yet unknown structure that is highly oriented on the substrate. Scanning electron microscopy images reveal small crystallites with uniform distribution on the surface. By investigating the structural stability under temperature load two changes in the properties of the MOF layer could be observed. At temperatures of 160°C and 300°C a change in the orientation of the crystallites could be detected. But more interestingly a reversible change of the lattice constant could be observed which can be attributed to a change of guest molecules in the MOF network.

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Keywords: MOF; Thin-films; X-ray diffraction

^{25&}lt;sup>th</sup> European Crystallographic Meeting, ECM 25, İstanbul, 2009 Acta Cryst. (2009). A**65**, s 298