

MS30 Advanced porous materials : MOFs, COFs, SOFs....and what else?

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Exploring the guest-induced structural dynamics in MOFs by in situ PXRD techniques

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Abstract

Metal-Organic Frameworks (MOFs) are crystalline porous solids, constructed from metal clusters and organic ligands, connected in 2D-Networks or 3D-Frameworks using the modular building principle [1]. Benchmark values of specific surface area and pore volume, but also target and precise design of pore aperture and its functionalization makes them quite promising for gas storage, separation, catalysis, sensors and many other applications [2]. Several dozens of MOFs show a unique feature of framework flexibility and can adapt their pore confinement upon adsorption and desorption of guest molecules, which is accompanied by the structural transitions in adsorbent [3, 4]. These solids are actively discussed for several applications, such as gas storage and separation, sensing and mechanical energy storage [5].

Monitoring the gas and vapour adsorption by PXRD allows to follow the structural changes of MOF and represents an important tool for the understanding of intrinsic framework dynamics. In the following contribution, we present multipurpose instrumentations, dedicated to monitoring the gas and vapour adsorption in MOFs by PXRD or X-ray absorption spectroscopy in a wide range of pressure and temperatures [6]. Instrumentations are commissioned at KMC-2 beamline of BESSY II synchrotron and are available for the users of the large scale facility. Several archetypical studies of guest-induced structural dynamics in micro- and mesoporous MOFs will be discussed.

However, the access to synchrotron instrumentation is limited and strongly connected to the beamtime proposals, work cycles of the large scale facility and other factors. This motivated us to develop *in situ* PXRD/adsorption chamber for the laboratory powder X-ray diffractometer. Herein, we introduce the instrumentation and the first results of PXRD studies using a laboratory *in situ* adsorption chamber.

References

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