Looking into microporous materials with solid-state NMR spectroscopy

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Preparing the most efficient microporous materials for catalysis, gas separation and storage, drug delivery etc. requires not only knowledge about the atomic-scale structures of these materials but also understanding of the atomic-scale processes during their action. In order to gain this knowledge and this understanding, it is mandatory that microporous materials are inspected by a set of complementary techniques that elucidate short- and long-range structural motifs, static and dynamic properties, interactions among the frameworks and the adsorbates. That is why, in addition to the very well established thermal, sorption and diffraction analyses, modelling and spectroscopic investigations are becoming more and more important in the studies of microporous materials.

Among the spectroscopic techniques, solid-state nuclear magnetic resonance is one of the most powerful characterization techniques, because it can provide element-specific atomic-resolution insight into materials. It can be used at many different stages of research connected to microporous materials; from studies of their formation, their structure determination, to in-situ studies of their performance. As a local spectroscopic tool, solid-state NMR is complementary to diffraction techniques that rely on the existence of long-range order and that provide a picture of an average crystal structure. NMR experiments can prove or disprove the hypotheses proposed by modelling, predicting preferential adsorption sites and estimating strength of interactions between the adsorbed molecules and the porous frameworks. It can follow gradual adsorption or desorption of molecules into pores, locate and quantify these molecules, and thus complement the data obtained by the thermal and sorption analyses. Solid-state NMR is also extremely important for studying dynamics of the frameworks and of the adsorbed molecules. Therefore, employing NMR spectroscopy is crucial for deducing the structure-to-function relationships.

In this contribution selected examples of the application of solid-state NMR spectroscopy for gaining an insight into the microporous materials will be presented. Particular attention will be devoted to deciphering motifs that do not exhibit long-range order and thus cannot be studied by diffraction.