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HOW TO FILL MOFS WITH DIFFERENT FLAVOURS

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The scope of this work is to find a systematic way to embed small molecular aggregates inside porous crystalline materials, with the multiple aims to explore the structural aspects of nanoconfinement, and of the stabilization of guest molecules inside the cavities of the structure. The feasibility of this approach stems from both the recent report that describes the structural determination of single molecules trapped inside a microporous framework [1] and the various reports showing the inclusion of species such as metal nanoparticles or polyoxometalates into mesoporous MOFs [2]. MOFs are highly versatile materials that are made by connecting metal ions with prefixed coordination geometry with rigid ligands acting as spacers, hence affording three-dimensional coordination polymers. The accurate design of the building units allows to design porous MOFs, obtaining cavities of considerable size, which usually accommodate loosely bound solvent molecules. The guest that we are considering here are some important compounds for the human health and nutrition which occur as liquids at room temperature, some organometallic precursors of inorganic oxides, and organometallic compounds potentially active in catalysis. We initially focused on a collection of already known MOFs, and we determined the interaction mode of some of the guests inside the pores (Figure 1), and the results will be shown. We then moved to the design of new organic linkers in order to better tune the topology and functionality of the MOF network. In particular, we aimed to decorate the inner cavities with hydrogen bond and halogen bond active functional groups, which could serve as anchoring points for the guests.

A small library of linkers was synthesized: one group is composed by flexible aminocarboxylic linkers, the second one is characterized by rigid amidic bonds and pyridine as coordinative function. These ligands were used for the synthesis of novel MOFs; due to the nature of the ligands these frameworks resulted quite flexible. Their structure and inclusion properties will be illustrated.

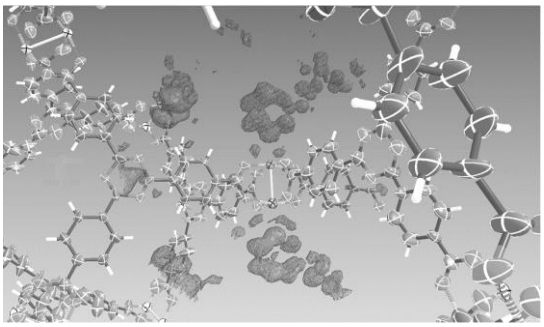

Figure 1. Experimental electron density of nicotine included inside the MOF known as PCN6 [3].

[1] Y. Inokuma et al., *Nature*, **2013**, *495*, 461–466
[2] C. Rösler, R. A. Fischer, *CrystEngComm*, **2015**, *17*, 199–217
[3] H.C. Zhou et al., *J. Am. Chem. Soc*,.**2007**, *129*, 1858-1859.