Structural analysis of Stimuli Responsive Metal-Organic Frameworks

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The material science of porous coordination polymers is one the most challenging research fields of materials chemistry during the last three decades. Among various representatives of such coordination compounds, an increasing attention has been devoted to metal-organic frameworks (MOFs), due to their advantageous possibility to link a wide range of metal ions or clusters with organic linkers, leading to 1-, 2- or 3-dimentional micro- or meso-porous networks. The large number of combinations between metal ions/clusters and organic linkers provide various types of functionalities (e.g. acid/base sites, hydrogen bonding sites or chiral sites) with adjustable porous properties. That is why, numerous MOFs have been intensively investigated as promising materials for gas storage and separation, sensing, catalysis, drug delivery, among other applications. The structure-property relationship plays a key role for the material science of porous frameworks. Very often fascinating phenomena upon gas adsorption can be either not well-understood (e.g. the switching of the gas selectivity), or missed out without in situ temperature/pressure variable experiments (e.g. negative gas adsorption). The monitoring of structural changes upon temperature/pressure/time-dependent adsorption is therefore of great importance for understanding the mechanisms of gas adsorption or separation. The goal of this project is to understand the structural behavior of a few representative robust MOFs using advanced temperature- and pressure-dependent single crystal and powder X-ray diffraction, in close relationship with *in-situ* infrared and another analytical methods of characterization of porous frameworks. The objective of this project is to synthesize and determine temperature-, pressure- and particle size-depended response of the MOFs materials developed at IMAP to the guest (e.g. CO_2, H_2O) uptake, in a view of potential applications in the field of CO_2 capture, dehumification or cooling systems, among other applications. Such fundamental studies requires the development of the (nano)structuration synthesis methods for the MOFs particles. This will be done through the synthesis platform available at IMAP (high-throughput, optimisation). Then, one will rely on the advanced X-ray diffraction methods, some of them being already available onsite (laboratory variable-temperature powder X-ray diffraction), while the others, such as synchrotron experiments or advanced single crystal X-ray diffraction will be organized via proposal application and/or will be developed at IMAP during the course of this PhD. Such advanced techniques will be combined with other methods such as thermogravimetric analysis, scanning electron microscopy, volumetric and gravimetric gas sorption isotherms, also available in the laboratory.

If you have a Materials Chemistry background, with a previous experience in materials synthesis and characterization (such as single crystal/powder X-ay diffraction) and wish to become a member of the IMAP team - welcome to visit https://adum.fr/as/ed/voirproposition.pl?langue=&site=edpcm&matricule_prop=53552#version or/and contact us.