**MS37 Advances in Structure determination of new materials by multi-technique approach including imaging techniques**

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# Structural elucidation of novel metal-organic frameworks using 3D electron diffraction

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Abstract

Metal-organic frameworks (MOFs) are hybrid crystalline porous solids demonstrating potential applications in different domains related to energy, environment or health [1]. The structural elucidation of nano-sized MOFs is essential as it provides a better understanding of their unique properties. However, the synthesis of robust MOFs often leads to polycrystalline compounds rendering the structure elucidation by single-crystal and powder X-ray diffraction often challenging. A good alternative is to solve the structure from 3-dimensional electron diffraction (3DED) data [2], a method allowing to solve the structure from much smaller particles by using electrons instead of X-rays.

Titanium-based MOFs (Ti-MOFs) are of interest due to their photoactive character, good biocompatibility and tunability in terms of pore engineering, which makes them attractive candidates in photocatalysis or energy-related reactions [3,4]. However, the design of new Ti-MOFs is still driven by serendipity due to the complexity of titanium chemistry in solution [5]. Here, we present a new robust nanoporous nitro functionalized titanium terephthalate MOF labelled MIP-209 (MIP stands for Materials from Institute of Porous Materials of Paris) constructed from Ti12O15 oxo-clusters, similarly to MIP-177 [1] as revealed first by X-ray Pair distribution function analysis (PDF). The structure has been then solved by ab initio methods using continuous rotation electron diffraction (cRED) data and refined kinematically.

In this communication, the structural characterization of MIP-209 by 3DED will be presented. in combination with complementary structural characterization methods such as pair distribution function (PDF) analysis and low-dose high-resolution TEM (LD-HRTEM). Due to the high electron beam sensitivity of MOFs, the latter was only made possible by the use of a microscope equipped with a direct detection electron counting camera (DDEC) [6], enabling the imaging of MOFs with low dose rates.

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Structural model (left) and HRTEM images (right).