**X-Ray Powder Diffraction Laboratory @ University of Málaga (UMA)**

Ángeles G. De la Torre,a Aurelio Cabeza,a Miguel A. G. Aranda,a,b Laura León-Reinac

*a Departamento de Química Inorgánica, Cristalografía y Mineralogía, Universidad de Málaga, 29071 Málaga, Spain. b* *ALBA synchrotron, Carrer de la Llum, 2-26, E-08290 Cerdanyola, Barcelona, Spain c* *Servicios Centrales de Investigación. Universidad de Málaga. 29071 Málaga, Spain* [mgd@uma.es](mailto:mgd@uma.es)

X-Ray Powder Diffraction (XRPD) laboratory is a facility placed at Servicios Centrales de apoyo a la Investigación (SCAI) at University of Malaga (UMA) http://www.scai.uma.es/. This facility has three XRPD diffractometers and a diffractometer to measure high-resolution thin-films.

X´Pert PRO MPD from PANalytical. This is a bragg-brentano (/2) with reflection geometry diffractometer which allows to obtain high resolution XRPD data with strictly monochromatic CuKα1 radiation (λ=1.54059Å) [Ge(111) primary monochromator] and an automatic sample charger. Moreover, it has parallel monochromatic CuKα1 radiation (λ=1.54059Å) with an hybrid Ge(220) monochromator for capillary and multiproposal (bulk samples up to 1 Kg) sample holders. The HTK1200N chamber from Anton Paar allows collecting high resolution high temperature patterns.

EMPYREAN from PANalytical. This diffractometer works in reflection and transmission geometries with / goniometer, using CuKα1,2 radiation (λ=1.5418Å), a focusing X-ray mirror and a ultra-fast PIXCEL 3D detector with 1D and 2D collection data modes (microstructural and preferred orientation analysis). Moreover, the TTK450N chamber allows low temperature and up to 450ºC studies.

A D8 ADVANCE (BRUKER) was installed in April 2014. It is the first diffractometer in Europe equipped with a Johansson Ge(111) primary monochromator, which gives a strictly monochromatic Mo radiation (λ=0.7093 Å) [1]. It works in transmission mode (with a sample charger) with this high resolution configuration. XRPD data suitable for PDF (Pair Distribution Function) analysis can be collected with a capillary sample holder, due to the high energy and high resolution capabilities of this diffractometer. Moreover, it has a humidity chamber MHC-trans from Anton Paar working on transmission mode with MoK (measurements can be collected at 5 to 95% of relative humidity (from 20 to 80 ºC) and up to 150ºC [2]). Furthermore, this diffractometer also has a reaction chamber XRK900 from Anton Paar (which uses CuKα1,2 radiation in reflection mode), which allows data collection from room temperature to 900ºC with up to 10 bar of different gases.

Finally, a D8 DISVOVER A25 from BRUKER was installed on December 2014. It has a five axis Euler cradler and optics devices suitable for high resolution thin film data collection collected in in-plane and out-of-plane modes. To sum up, high-resolution thin films, microstructural, rocking-curve, Small Angle X-ray Scattering (SAXS), Grazing incident SAXS (GISAXS), Ultra Grazing incident diffraction (Ultra-GID) and microdiffraction measurements can be performed with the appropriated optics and sample holders.

[1] L. León-Reina, M. García-Maté, G. Álvarez-Pinazo, I. Santacruz, O. Vallcorba, A.G. De la Torre, M.A.G. Aranda “Accuracy in Rietveld quantitative phase analysis: a comparative study of strictly monochromatic Mo and Cu radiations” *J. Appl. Crystallogr.* **2016,** 49, 722-735.

[2] J. Aríñez-Soriano, J. Albalad, C. Vila-Parrondo, J. Pérez-Carvajal, S. Rodríguez-Hermida, A. Cabeza, F. Busqué, J. Juanhuix, I. Imaz, Daniel Maspoch “Single-crystal and humidity-controlled powder diffraction study of the breathing effect in a metal-organic framework upon water adsorption/desorption” *Chem. Commun., 2016,* DOI: 10.1039/C6CC02908F.