PhD- position in Grenoble and Madrid

In situ and PDF neutron diffraction for the advanced structural analysis of MOF catalysts for carbon dioxide valorization

This PhD project focuses on the advanced structural characterization of two families of MOFs with the use of neutron diffraction techniques, to unveil some of their unique features, as well as their behavior during the catalytic processes. In particular, it is proposed the use of pair distribution function (PDF) analysis of neutron diffraction data to elucidate the possible atomic arrangements of various elements in multimetal MOFs, which is not achievable with traditional methods. In addition, the structural changes and the guest-framework interaction of MOFs with in situ neutron powder diffraction studies will be investigated. Neutron diffraction data of the MOFs under controlled environments will be acquired and analyzed to describe the role of the different framework components during the catalytic cycles. The knowledge acquired with these studies will be used to correlate the catalytic properties of the materials with their complex structural features, allowing the devise of novel generations of advanced materials for carbon dioxide catalytic valorization.

We are looking for a highly motivated candidate to be part of a project focused on the use of neutron diffraction techniques for advanced structural analysis of MOF based catalysts. We offer a 3-year contract to complete a joint PhD between ILL (France) and the Materials Science Institute of Madrid (Spain). The contract is funded through the MCIN / ILL scientific member agreement.

Candidates must hold a MSc degree and meet the requirements to be enrolled in a Chemistry PhD program. Previous knowledge on crystallography and use of diffraction techniques will be valuable. For further information and to submit your application (CV and motivation letter), please contact Inés Puente-Orench (<u>puenteorench@ill.fr</u>), Felipe Gándara (<u>gandara@icmm.csic.es</u>) and Gabriel Cuello (<u>cuello@ill.fr</u>).

Deadline 30th January 2023