NÉEL INSTITUTE Grenoble

Topic for Master 2 internship – Academic year 2019-2020

Low-dose EDT for highly sensitive MOFs

General Scope:

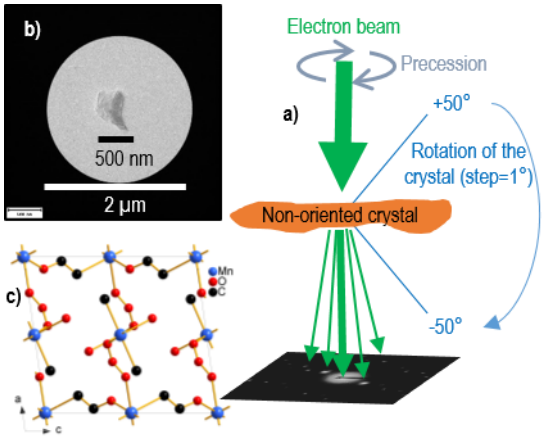
Metal-organic frameworks (MOFs) are materials that can be tailored for their structure and properties by assembling organic functional molecules with metal atoms. The wide range of different MOFs have enabled their use in numerous applications including catalysis, storage of fuels (hydrogen, methane), capture of carbon dioxide, proton conductors for fuel cells, photovoltaics, sensors and electronic materials. In recent years, there is an almost exponential increase of MOF structures in the Cambridge Structural Database (CSD) so that there is no doubt that they will be one of the most important material classes for innovation in the future. The development of these materials is closely dependant on structural characterizations but for most MOFs it is notoriously difficult to obtain large enough crystals of sufficient quality for X-ray structure analysis. Thus, there is a great number of highly interesting compounds that have not yet been studied because of the difficulty of determining their structures. We have recently developed a low-dose electron diffraction tomography (LD-EDT) technique that is well adapted to such difficult materials. In this internship the student will be trained to use the TEM and to apply LD-EDT to different MOFs. The goal is to optimize the experimental parameters of the technique and to solve the structures of relevant MOFs synthesized by our collaborators in Lyon.

Research topic and available facilities:

The goal of this internship is to apply low-dose electron diffraction tomography to study the atomic structure of these sensitive materials. The internship will include several stages:

- Performing electron diffraction experiments under these conditions on MOFs in order to solve their structures.
- Investigation of the optimal experimental conditions yielding the highest quality structure solutions.
- Solving the structures of MOFs from the LD-EDT data.

In the framework of a collaboration the MOFs are synthesized by D. Luneau in Lyon and will be studied for their structure in the Néel Institute. The intern will be trained in the use of the transmission electron microscope of the Néel Institute. He/she will acquire diffraction data and perform the complete data treatment using specific computer programs that are available at the Néel Institute, which should lead to the resolution of the structures.



Possible collaborations and networking:

The intern will be integrated into the electron microscopy group of the Néel Institute. He/she will collaborate with the chemists that synthesize the materials and the X-ray crystallographers of the Néel Institute.

Possible extension as a PhD: Yes.

Education / Required skills: Master in Physics, Solid state chemistry, instrumental physics. Basic knowledge in crystallography and diffraction

Start date: 2020

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