INSTITUT NEEL Grenoble

PhD grant

The structure of coordination polymers studied by electron crystallography (3D-ED)

Context:

Coordination polymers are materials whose structure is made up of organic molecules and metal atoms. Their structures and thus properties can be controlled by the choice of molecules and metal atoms used and the possible variations of these materials are therefore virtually infinite. They can be found in a wide variety of applications: catalysis, fuel storage (hydrogen, methane), carbon dioxide capture, proton conductors for fuel cells, photovoltaics, sensors and electronic materials.

The development of these materials and a detailed understanding of their properties is highly dependent on the ability to accurately determine their crystallographic structures. However, for most coordination polymers, it is notoriously difficult to obtain crystals of sufficient size and quality for structural determination by X-ray diffraction. As a result, a large number of potentially interesting compounds remain unexploited due to the difficulty of studying their structures.

Objectives and means available:

The aim of this thesis project is to solve the structures of coordination polymers using electron crystallography, and thus make a significant contribution to the search for new materials in this field. In this thesis project, we will use electron diffraction, since for this technique nanometric crystals are sufficient for solving the structures. A combination of methods and strategies from structural biology and materials science will enable us to optimize data acquisition and processing.

For his/her research work, the PhD student will be integrated into the Institut Néel's MRS team. He/she will carry out 3D electron diffraction experiments on the state-of-the-art transmission electron microscope (TEM) (commissioned in 2022), equipped with a direct-detection camera and a fast C-MOS camera, as well as a module for precession-mode electron diffraction. The Institut Néel's transmission electron microscopy platform also includes a dedicated sample preparation area. The software required for data processing is also available in the laboratory. The synthesis of MOF materials will be carried out by our collaborators in Lyon.

The thesis will comprise several stages:

- Performing electron diffraction experiments in a transmission electron microscope under low-dose conditions on coordination polymers.
- Optimization of experimental conditions to obtain diffracted intensity sets of the highest quality.
- Combining data processing methods from structural biology and materials science.
- Structural resolution of coordination polymers from 3D ED data.
- Structure refinement from 3D ED and/or X-ray powder diffraction data.

Possible collaboration and networking:

The collaboration with Dominique Luneau (LMI, Université Claude Bernard Lyon 1) concerns the synthesis of new coordination polymers with two- or three-dimensional structures for which structure determination by X-ray diffraction is not possible (ANR MagDesign in progress), as well as measurements of the compounds' magnetic properties.

Collaboration with Dominique Housset and Wai Li Ling (IBS, Grenoble) involves the pooling of crystallographic methods from the fields of structural biology and materials science. The synergy created by combining methods from both communities enables us to solve previously inaccessible structures.

Required profile:

- Master in Physics, Solid state chemistry or instrumental physics.
- Basic knowledge in crystallography and diffraction
- Knowledge in transmission electron microscopy would be appreciated

Foreseen start for the grant: October 2024 **Duration**: 36 months

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