INSTITUT NEEL Grenoble

PhD grant

Understanding processing-structure-property relationships in New Energy materials design by Full Structure determination

Context :
Structural disorder and sample nanostructuration are increasingly being attributed to desirable physical phenomena in functional materials with a diverse range of exploitable properties. When determining the structure of disordered and nanostructured materials we need to go beyond crystallography, limited to the average structure, to delve into the understanding of correlated disorder. A successful solution lies in the convergence of experimental, computational and algorithmic approaches to combine theory and the simultaneous refinement of multiple datasets.
The student will acquire the expertise to combine multiple experimental inputs with different element and length-scale sensitivities, namely Pair Distribution Function (PDF) analyses, total scattering, and core spectroscopies. The student will liaise with scientists pioneering new synthetic approaches including mechanochemistry, severe plastic deformation or flash sintering for the development of new energy materials for hydrogen storage and all-solid-state battery applications. The student will also design new multi-modal sample environments to investigate the performance of these energy materials *operando*.

Objectives and means available :
The student will acquire valuable skills at the chemistry lab including a range of processing techniques. The student will perform basic characterizations to aid the fundamental understanding of the systems investigated that they will also adapt for operando characterisations at large scale facilities using both synchrotron X-rays and neutrons.
The student will be based at the 'Matériaux, Rayonnements, Structure' group (MRS) the focus of which is to correlate structure-property relationships of a wide spectrum of complex materials (e.g., multiferroics, inhomogeneous materials, alloys...). The Institut Néel will provide access to some of the most complex structural problems of relevance to current materials research. The student will be supervised by M. Diaz-Lopez and work within the MRS group with L. Laversenne and P. de Rango, and the French Cooperative Research Groups at the nearby ESRF and ILL.

Possible collaboration and networking :
The student will cooperate with a multidisciplinary team (chemists, material scientists, beamline technicians and beamline scientists) to drive this project to completion. The supervisor will support the student's learning with regular discussions to encourage teamwork, as well as to motivate and encourage input from the student. International travel to perform experiments at leading world-class large-scale facilities and conferences is expected.

Required profile :

- This project is suitable for students' following degrees in the following broad subjects: Chemistry, Materials Science or Physics,
- The candidate should have a hands-on attitude.
- Experience with working on a multidisciplinary team is desirable.
- Creative thinking and problem solving.
- The student should have a basic understanding of characterization techniques in material science from a previous undergraduate or master project: sample morphology studies by SEM, (im)purity fingerprint assessment with X-ray diffraction.
- Communication and leadership

Foreseen start for the grant : September/October 2023
Duration : 36 months

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