



In the framework of a European project, CEA-IRIG and IM2NP are seeking to recruit a:

PhD position: Watching catalysts at work with Bragg coherent diffraction imaging

The CEA-Grenoble (cea.fr) is a major French research organization. CEA-IRIG ([irig](http://irig.cea.fr)) is one of its institutes, dedicated to fundamental research. It is located within the Minatec (minatec.org) campus. IM2NP ([IM2NP](http://im2np.fr)) is a well-recognised research center in materials science, nanoscience, and microelectronics, based in Marseille. The European synchrotron ([ESRF](http://esrf.eu)) is one of the world's leading international synchrotron facilities.

The Subject

This PhD thesis is part of the European-funded project REACT (*REvolutionising the use of coherent X-ray diffraction for structural crystallography Applied to CaTalysis*), which aims to apply advanced coherent diffraction imaging capabilities (1, 2) to watch nanostructures at work. The project focuses on studying the structural evolution of individual nanocrystals during their operation (mainly catalytic reactions). Using the unique capabilities of Bragg coherent x-ray diffraction imaging (BCDI), it is possible to map *in situ* and *operando* the three-dimensional evolution of the composition, deformation/strain field and crystallographic defects of nanocrystallites to get a comprehensive experimental structure-performance relationships with a spatial resolution as low as 5 nm. Experiments will be carried out mainly at the European synchrotron (ESRF) in a leading international scientific environment. The project also involves close collaboration with IM2NP in Marseille, a center renowned for its expertise in materials characterization.

The function

This PhD thesis aims to uncover fundamental surface structure-property relationships by exploiting the unique capabilities of BCDI. The successful candidate will investigate, *in situ* and *operando*, the structural evolution of catalytic nanoparticles during operation. They will gain hands-on experience with state-of-the-art synchrotron x-ray techniques, catalytic reaction setups, and advanced data analysis methods. The project will focus on obtaining time-resolved three-dimensional maps of nanoparticle composition and lattice strain under working conditions. Atomistic simulations will be used to validate and interpret the experimental results. Together, these approaches will enable detailed analysis of the internal structure of nanoparticles and provide insights for their optimization under operating conditions.

Profile of the applicant

The applicant should have a strong background in materials science, condensed matter physics, physical chemistry or chemistry. X-ray coherent diffraction imaging is based on so-called reconstruction algorithms. The student should have experience or shows some interest in learning data analysis and analysis program development using e.g. Python programming. Experience in crystallography and Python programming will be considered an asset. He/she should have good interpersonal, communication, organisational and presentational skills.

Contract

The PhD position will be located at the ESRF in Grenoble. The PhD candidate will be under the supervision of Dr. Stéphane Labat (IM2NP) and Dr. Marie-Ingrid Richard (CEA-Grenoble). The application should include a statement of research interest, a CV and Master's degree transcript to be sent to Stéphane Labat (stephane.labat@univ-amu.fr) and Marie-Ingrid Richard (mrichard@esrf.fr).

1. M. Dupraz *et al.*, *Nat. Commun.* **13**, 3003 (2022).
2. C. Atlan *et al.*, *Nat. Mater.* **22**, 754–761 (2023).