INSTITUT NEEL Grenoble

Post-doctoral position

Development of a novel 3D hyperspectral X-ray nanoimaging methodology for the characterization of technical catalysts

Context:
This 18-months postdoctoral project is funded by an ANR (French National Research Agency) JCJC project, entitled "Adding Spectral capabilities to ptychographic imaging of Technical Catalyst". The innovation of this project is the combination of 3D X-ray phase-contrast imaging via ptychography and spectroscopic techniques to give rise to a novel 3D hyperspectral nanoimaging. This methodological develop will have an immediate impact in the catalysis industry by enabling the characterization of technical catalysts at different life stages. Progress in catalysis has always been motivated by societal needs, such as environment, energy, and fuels, with the goal of improving the efficiency of the catalytic process on a technical scale. Technical catalysts are complex multicomponent bodies, ranging from dozens of μm to several cm, consisting of active phases, supports, and additives in shaped forms suitable for their application. They differ strongly from a research catalyst, i.e., the laboratory-developed materials constituted by a single bulk or supported active phase, which is the predominant focus of academic investigations. Yet despite the tremendous relevance, understanding the complexity of their structure-property-function relationships is very challenging, mainly due to the limitations of the characterization techniques. Ptychographic X-ray Computed Tomography (PXCT) is a 3D X-ray nanoimaging technique that overcomes these shortcomings and has revolutionized the characterization of technical catalysts (Fig. 1). However, access to the localization and state of individual chemical elements within the sample structure is not yet directly possible. By adding spectral capabilities to ptychography and PXCT, this project aims at bridging this gap between the morphological and spectroscopic characterization of technical catalysts.

Objectives and means available:
The main goal of this postdoctoral project is the methodological development of a novel high-resolution 3D hyperspectral imaging for the characterization of technical catalysts by combining X-ray computed tomography and spectral-ptychography. The addition of spectral capabilities to ptychography will provide information about the locations and the chemical state of the metals that promote or poison the catalysts within the 3D microstructure. Two modalities will be implemented: 1) Resonant imaging and 2) Near-Edge Structure spectroscopic imaging. High-performance computing resources will be available and Python-based software will be developed for simulation, data analysis, 3D image rendering, and segmentation. Machine and deep learning will be also used for data analysis and segmentation.

Possible collaboration and networking:
She/he/they will collaborate with scientists and engineers from NÉEL Institute CNRS/UGA, French CRG beamlines at ESRF, and KAUST catalysis center (KCC), Saudi Arabia. Working trips to different synchrotron source facilities for data collection will be organized. Additionally, Grenoble is an important scientific hub hosting important research institutions and technological companies.

Required profile:
- PhD in Physics, Chemistry, Materials Science, Electrical Engineering, or closely related science obtained less than 2 years ago.
- Good background in X-ray spectroscopy and/or X-ray imaging.
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- Programming skills, including method development and imaging processing, are highly desirable and important for the development of this project.
- Experience with catalysis is considered an asset.
- English proficiency is necessary and French is considered an asset.

**Duration**: 18 months

**Salary**: According to the university/CNRS salary grid for a Postdoc (~2600 euros/month gross).

**Foreseen start for the position**: January/2021

Applicants should send a CV, a motivation letter, and at least one referee (or recommendation letter if available already) contact to:

**Contact**: Julio Cesar DA SILVA  
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