CEA-Grenoble/IRIG is seeking to recruit a:

PhD student (f/m): Unveiling CO_2 reduction reactions: nanoparticle insights *via in situ* & *operando* Bragg coherent x-ray imaging

The CEA-Grenoble (cea.fr) is a major French research agency and IRIG (Irig) is one of its institutes, devoted to fundamental research, in the Grenoble Minatec (Minatec.org) area.

The Subject

The imperative to capture and convert CO_2 into value-added chemicals or fuels represents one of the most significant challenges in achieving a sustainable society. The conversion of CO_2 into hydrocarbons is considered a highly promising avenue, as it not only mitigates the greenhouse effect but also offers a means of storing energy by transforming intermittently available renewable electricity into chemicals. This project aims to investigate the structural evolution of individual nanocrystals during CO_2 reduction reactions. Using the unique capabilities of Bragg coherent X-ray imaging and phase retrieval algorithms [1], we can dynamically map, *in situ* and *operando*, the three-dimensional changes in lattice deformation, strain, composition, and crystallographic defects of nano-crystallites, establishing a comprehensive experimental framework for structure-performance relationships.

The Function

The aim of the thesis is to extract, from structural information (morphology, strain field, crystallographic defects, oxidation state) obtained for catalysts, a mechanistic understanding to render CO_2 reduction catalysts both efficient and selective. For example, in Cu alloy nanoparticles, the products of CO_2 reduction are closely linked to the surface and subsurface chemical composition of the catalyst. By controlling the alloying ratio, chemical bonds as well as electronic properties can be tuned to influence the binding energy of CO_2 reduction intermediates. The application of 3D coherent diffraction imaging with nano-spectroscopy should pave the way for analysing the internal structure of nanoparticles and their optimisation during catalytic reaction. Code development using Python is expected during the project. Experiments will be primarily conducted at the ESRF, the European synchrotron located in Grenoble near CEA-Grenoble, in a leading international scientific environment. The project will be in collaboration with LEPMI (Laboratory of Electrochemistry and Physico-chemistry of Materials and Interface, Grenoble-France), which has a strong expertise in electrocatalysis, materials science, and energy storage and conversion systems.

Profile Of The Applicant

The applicant will be in possession of a Master in Sciences. 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. She/he should also show interest in electrochemistry. He/she should have good interpersonal, communication, organisational and presentational skills.

Contract Characteristics

The PhD candidate will be under the supervision of Dr. Marie-Ingrid Richard (CEA-Grenoble, visiting scientist at ESRF) and Dr. Frédéric Maillard (LEPMI). The office will be located at ESRF, Grenoble.
Interested applicants should submit:
(1) 1 page cover letter stating his/her motivation,
(2) curriculum vitae,
to Marie-Ingrid Richard (mrichard@esrf.fr) and Frédéric Maillard (frederic.maillard@lepmi.grenoble-inp.fr). Deadline: June, 10th 2024.

[1] C. Atlan et al., *Imaging the Strain Evolution of a Platinum Nanoparticle under Electrochemical Control*, Nat. Mater. **22**, 6 (2023).