Grenoble INP - UGA is a renowned public institution of higher education and research, and a major player in the Grenoble ecosystem. It is the engineering and management institute of Grenoble Alpes University, and plays a leading role in the scientific and industrial community.

### Researcher in Coherent X-ray Diffraction Imaging

<table>
<thead>
<tr>
<th>Job ad reference</th>
<th>2023-RESEARCHXRAYDIFF-LEPMI</th>
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<tbody>
<tr>
<td><strong>Research field</strong></td>
<td>Electrochemistry / Materials science / Coherent X-ray diffraction 3D reconstruction of palladium nanoparticles during hydrogen insertion/de-insertion via coherent X-ray diffraction</td>
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<tr>
<td><strong>Host laboratory</strong></td>
<td>Laboratory of Electrochemistry and Physicochemistry of Materials and Interfaces (LEPMI, UMR 5279 Grenoble-INP, UGA and CNRS)</td>
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<td><a href="https://lepmi.grenoble-inp.fr/">https://lepmi.grenoble-inp.fr/</a></td>
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<td><strong>Requested profile</strong></td>
<td>Recognised researcher (R2)</td>
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<tr>
<td><strong>Location</strong></td>
<td>Saint Martin d’Hères (Grenoble, France)</td>
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<tr>
<td><strong>Date of recruitment / contract term</strong></td>
<td>08/01/2024 (6 months contract)</td>
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<tr>
<td><strong>Contacts</strong></td>
<td>Dr. Frédéric Maillard <a href="mailto:frederic.maillard@grenoble-inp.fr">frederic.maillard@grenoble-inp.fr</a></td>
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Grenoble INP - UGA is a leading public institution accredited with the French label “Initiative d’excellence”. It offers innovative engineering and management programs, with an increasing internationalization of its course offers. The courses are grounded in sound scientific knowledge and linked to digital, industrial, organizational, environmental and energy transitions. The Engineering and Management Institute of Grenoble Alpes brings together more than 1300 staff members (teacher-researchers, lecturers, administrative and technical staff) and 8300 students, located on 8 sites (Grenoble INP - Ense3, Grenoble INP - Ensimag, Grenoble INP - Esisar, Grenoble INP - Génie industriel GI, Grenoble INP - Pagora, Grenoble INP - Phelma, Polytech Grenoble, Grenoble IAE and the INP Prepa). Grenoble INP is also a highly-ranked institution of higher education and research, leading the way in the fields of engineering and management on an international scale. It is a member of a large number of international academic and research networks. It is part of the European University UNITE! As part of Grenoble Alpes University, Grenoble INP has associated guardianship of 39 national and international research laboratories and of technological platforms. The research conducted there benefits both its socio-economic partners and its students. Grenoble INP is at the heart of the following scientific fields: physics, energy, mechanics and materials; digital; micronanoelectronics, embedded systems; industry of the future, production systems, environment; management and business sciences.

Grenoble INP - UGA is an equal opportunity employer committed to sustainability. Grenoble INP-UGA celebrates diversity and equity and is committed to creating an inclusive environment for all employees. All qualified applications will be considered without discrimination of any kind.

**Research**

LEPMI ([https://lepmi.grenoble-inp.fr/](https://lepmi.grenoble-inp.fr/)) is a joint CNRS - Grenoble INP - UGA - Université Savoie Mont-Blanc research unit with about 100 researchers. Its research interests concern the storage and electrochemical conversion of energy, and combine electrochemistry, materials science and electrochemical engineering.

The post-doctoral fellowship will be carried out in the Interfacial Electrochemistry and Processes (EIP) team of LEPMI under the supervision of Dr. Frédéric Maillard.

The EIP team counts 16 permanent researchers and 30+ PhD/postdoc students. It is internationally recognized for its expertise in electrocatalysis and elucidation of degradation mechanisms of fuel cell and electrolyzer catalysts.

**Job description :**

Within the framework of the European projects HERMES and CARINE, LEPMI and the Institute for Interdisciplinary Research of Grenoble (IRIG) are interested in the insertion and de-insertion of hydrogen (H) in palladium (Pd) nanocrystallites (NCs). To date, the mechanisms and kinetics of Pd hydride nucleation (preferential sites for nucleation or homogeneous nucleation over the entire surface of CNs) and phase transformation (coexistence of two phases or homogeneous transformation) remain open questions. A unique method in the world to obtain this information under operando conditions (i.e. in the liquid phase, under potential control) is coherent X-ray diffraction under Bragg conditions (BCDI).

The objective of this post-doctoral project will be to reconstruct in 3 dimensions using coherent X-ray diffraction images several Pd NCs during the electrochemical absorption/desorption of H2. The post-doctoral fellow recruited at LEPMI will process the signals using interactive algorithms. A first challenge will be to reconstruct simultaneously two separated Bragg reflections in Fourier space (reciprocal space). During phase transformation by hydridation, two phases (the α and β phases of PdH) can coexist in an individual Pd NC. The 3D diffraction images of the different phases can be reconstructed individually. But it will be crucial to reconstruct them simultaneously in order to spatially locate these phases in the NC. A second challenge will be to reconstruct highly-strained NCs. At low H concentrations, the maximum solubility of H is reached in the α phase. A further increase in H concentration is accompanied by a transformation to β phase, with a different lattice parameter.
The difference in lattice parameter between these phases is 3.5%, which induces significant strain during \( \alpha \) to \( \beta \) phase transition. The question of the convergence of the algorithm for deformed NCs will then be of major importance. Different combinations of iterative algorithms will need to be tested with constraints (such as a constant electron density value, the phase gradient, the phase symmetry indicated by the symmetry of the system, etc.). We hope to identify the most appropriate algorithmic solution for highly deformed nanocrystals. The algorithms will be made open source. A third challenge will be to improve the visualization of the reconstructed data, their homogeneous and heterogeneous deformation, as well as the average lattice parameters obtained during reconstruction.

The work of the post-doctoral fellow will be combined with \textit{ab initio} calculations carried out in the team of Dr. Marie-Ingrid Richard, research director at the CEA Grenoble.

**Specific requirements or conditions**

- Skills in materials science and more specifically X-ray diffraction are a pre-requisite,
- Ability to work in a team,
- Ability to synthesize/react to reports/publications
- Ability to code in Python
- Proficiency in English and French

**Specifics of the position**

Coherent X-ray diffraction measurements will be carried out during measurement campaigns at the European Synchrotron Radiation Facility (ESRF). They last from 48 to 120 hours in relays of 2 to 3 people day and night.

The post-doctoral fellow will work between three sites: LEPMI Grenoble, CEA Grenoble and ESRF.

**Position assigned to a restricted area: YES**

(Device for the protection of the scientific and technical potential of the nation, conditioning the appointment of the researcher to the authorization of the Defense Security Officer).

**How to apply**

Applications must be sent to: frederic.maillard@grenoble-inp.fr

Application deadline: 08th November 2023