

# Postdoctoral Appointee – AI/ML for X-ray diffraction

## Missions

In many fields, such as the fight against climate change, medicine, information and communication technologies, making advances requires continuous discovery of new inorganic materials. In this context, our primary objective is to accelerate the search for new materials, through a methodology that relies on prediction and characterization methods. Through our partners in Sorbonne Université, and Synchrotron Soleil, crystallization sequences followed by *in situ* XRD of diverse ternary and quaternary compounds are collected. The objective of the postdoctoral researcher at IMN will be to develop tools to automatically analyze the crystallization sequences for the identification of known and unknown phases and to use machine learning algorithms to assist the chemists towards the synthesis of pure new materials.

## Activities

The postdoctoral researcher will be responsible for implementing machine learning tools for X-ray diffraction. This will involve:

- Developing tools for the automatic identification of diffraction patterns of each phase present in a crystallization sequence using non-negative matrix factorization and clustering.
- Automated identification and quantification of these phases.
- Using deep learning algorithms, such as LSTM, and Bayesian optimization to guide the synthesis of pure materials.

## Expected Skills

### *Basic Qualifications:*

- PhD in materials science, chemistry, physics, or computational sciences
- Experience with X-ray science techniques (e.g., tomography, diffraction, etc.).
- Software development practices and techniques for computational and data-intensive science problems.
- Comprehensive experience programming in Python.
- Communication skills, ability to communicate effectively with internal and external collaborators and ability to work in team environment.

### *Preferred Qualifications:*

- Experience with machine learning methods and deep learning frameworks.
- Experience on applied machine learning (e.g., successful projects that used ML to resolve scientific problems).
- Experience and skills in interdisciplinary research involving computer and material scientists.

## Context

The Institut des Matériaux de Nantes Jean Rouxel (<https://www.cnrs-imn.fr/>) brings together more than 150 researchers and doctoral students. Through the design and characterization of new materials, the laboratory's approach aims to optimize a wide range of properties for applications such as photovoltaic cells, fuel cells, batteries for electric vehicles, nanotechnologies, and optical materials like LEDs. The MIOPS team, where the

work will be conducted, specializes in the synthesis and characterization of inorganic and organic-inorganic hybrid materials with optical, optoelectronic, or magnetic properties. The contract is funded by PEPR DIADEM.

**Salary**

Between €3021 (without experience) and €4208 (up to 7 years of experience) gross per month, depending on experience.

**Duration**

Minimum 18 months.

**Contact**

David Berthebaud (David.BERTHEBAUD@cnrs-imn.fr)

Romain Gautier (Romain.Gautier@cnrs-imn.fr)

Olivier Hernandez (Olivier.HERNANDEZ@cnrs-imn.fr)