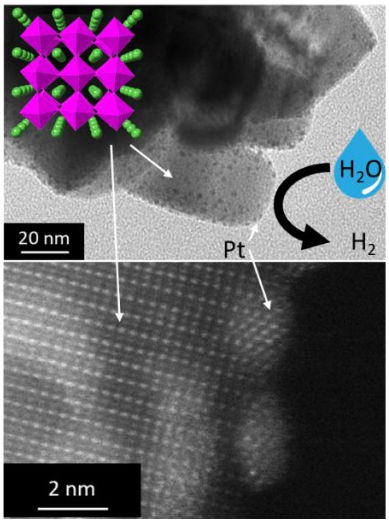
Master thesis proposal

Real-space structural assessment of local disorder in inorganic materials

Keywords: X-ray scattering, pair-distribution function, nanomaterials characterization, machine learning

SCIENTIFIC DESCRIPTION:

Atom-scale disorder and interfaces in inorganic materials are often the origin of unique properties applied from sensors and quantum computing to catalysis, energy conversion and storage. Identifying the nature of these deviations to the ideal crystal structure is a challenge because most methods, like X-ray diffraction (XRD), probe the ordered structure. To grasp these features, Pair Distribution Function (PDF) analysis has emerged few years ago.[1,2] From an XRD pattern, it provides the distribution of distances between all pairs of atoms, yielding local information on amorphous powders and defects in crystalline materials, which is inaccessible from regular XRD analysis. However, identifying local atomic environments from an experimental PDF requires fitting versus an initial structural model. This step is often the bottleneck of PDF analysis, as little experimental data are available to support the model and classical crystallographic considerations are not sufficient. To cope with this challenge, an approach has recently emerged, coupling experimental PDF data with machine learning (ML-MotEx) and the Atomic Simulation Environment python packages to deliver detailed models unachievable otherwise.[3]



Our goal in this project is to fathom a methodology to accelerate PDF analysis of materials, using the above-mentioned AI-based tools, thus enabling analysis of PDF data recorded *ex situ* but also *in situ* during reactions. We will first study the "textbook case" of perovskite Pt-doped $SrTiO_3$ nanocrystals that undergo exsolution of Pt nanoparticles by thermal treatment under reductive atmosphere. The process yields ~1 nm Pt clusters (too small for regular XRD analysis, see transmission electron microscopy images in the Figure) epitaxially bonded to the surface of 20 nm $SrTiO_3$ nanoparticles. The resulting material is an original electrocatalyst of hydrogen production from acidic water electrolysis. PDF will enlighten structural changes and local strains in the perovskite, in the clusters and at interfaces. We will further move to the analysis of quaternary non-oxide compounds developed in the frame of the national MADNESS project of PEPR MADNESS, for hydrogen production from alkaline water electrocalysis. These materials predicted by generative AI methods were recently produced experimentally. We will use PDF to provide information on substitutional disorder, which cannot be addressed by AI methods used for structure prediction.

[1] S. Billinge, **Phil. Trans. R. Soc. A.** 377 :20180413 (2019). Link
[2] Y. Song, C. Sassoye, D. Portehault *et al.* **Journal of the American Chemical Society**, 145, 19207 (2023). Link
[3] A. S. Anker et al., **npj Comput Mater**, 8,1 ,213 (2022). Link

Methods in use: Laboratory and synchrotron-based (SOLEIL CRISTAL and DIFFABS beamlines) XRD and PDF, machine learning (ML-MotEx) and ASE python packages for data analysis, synthesis of inorganic materials using already set protocols.

Budget description and use: 6 months internship: 3900 €, travels for synchrotron exp: 400 €, lab. synthesis (chemicals) and characterization (XRD, PDF): 700 €. Total: 5000 €

Applicant skills: Knowledge in materials science, willingness to learn Python code

Industrial partnership: N

Internship supervisors: Capucine SASSOYE, capucine.sassoye@sorbonne-universite.fr; David PORTEHAULT, david.portehault@sorbonne-universite.fr , website: https://david-portehault.lcmcp.science

Internship location: Lab. Chimie de la Matière Condensée de Paris, Sorbonne Université, Jussieu

Possibility for a Doctoral thesis: Possibility to apply for doctoral school funding (ED397).