As part of the DIADEM (Integrated Devices for Accelerating the Deployment of Emerging Materials) PEPR project, CEA-Grenoble/IRIG is seeking to recruit a:

Post-Doctoral Fellow (f/m): Workflow development for nano-imaging, atomistic simulations & machine learning applications

The Subject

The rapid discovery of functional materials is essential. Materials are becoming increasingly complex, with a considerable number of parameters to be taken into account in order to synthesise, characterise and optimise their structural or functional properties. CEA-Irig is developing new coherent diffraction imaging (CDI) methods to probe the structure of nanomaterials in three dimensions and non-destructively with a spatial resolution of 5 nm^3, even during their catalytic reactions [1,2]. We aim to develop and apply machine learning (ML) and, more generally, data science approaches for advanced imaging and characterisation of nanoscale systems. Experiment is nothing without simulation. We will take advantage of the new atomistic potentials to understand the full picture of catalytic mechanisms at work. We aim to develop a fully integrated workflow that combines experimental CDI data with simulations, such as molecular statics or dynamics. In addition, the “phase retrieval" problem - central to CDI - often relies on iterative algorithms that may not converge reliably. ML will be applied to different tasks such as phase retrieval, super-resolution, and phase unwrapping to unambiguously reverse the diffraction patterns and image 3D structures at nanometer resolution.

The Function

The project will be conducted in close collaboration with the ID01 beamline at The European Synchrotron (ESRF), a world-leading X-ray facility located in Grenoble, France. The candidate will first develop a workflow that integrates experimental coherent diffraction imaging data with atomistic simulations (either static or dynamics - using interatomic potentials, possibly developed by AI). Subsequently, ML will be applied in various areas: (1) enhancing the phase retrieval process through tasks such as super-resolution, denoising, phase unwrapping and phase retrieval itself; (2) identifying characteristic features in diffraction patterns, including crystallographic defects [3]; and (3) evaluating the algorithm’s performance on real datasets collected by CEA-Irig at ESRF, while analysing any performance improvements. The developed tools will be packaged in containers for streamlined deployment.

Profile Of The Applicant

The candidate should have a PhD in physics, materials science, computer science or a closely related science. We expect the candidate to have a broad interest in computer science and machine learning as well as a good background in physics and mathematics (linear algebra, numerical methods, statistics). The candidate should have very good programming skills (Python). He/she should have good interpersonal, communication, organisational and presentational skills.

Contract Characteristic s

This is a **2-year** contract located at Grenoble (CEA & ESRF). Interested applicants should submit: (1) 1 page cover letter stating the motivation, research experience and goals, and anticipated available date; (2) curriculum vitae, and (3) contact information for 2 references (reference letters are not required at this time)
to Marie-Ingrid Richard (mrichard@esrf.fr) and Thierry Deutsch (Thierry.Deutsch@cea.fr).

[1] M. Dupraz et al., Imaging the facet surface strain state of supported multi-faceted Pt nanoparticles during reaction, Nat. Commun. **13**, 1 (2022). [2] C. Atlan et al., Imaging the strain evolution of a platinum nanoparticle under electrochemical control, Nat. Mater. **22**, 6 (2023). [3] B. Lim et al., A convolutional neural network for defect classification in Bragg coherent X-ray diffraction, Npj Comput. Mater. **7**, 1 (2021).