

PostDoc/Research Software Engineer at LSMO EPFL

DESCRIPTION

X-Ray photoelectron spectroscopy (XPS) is a surface characterization technique that allows the analysis of the topmost nanometers of a material. XPS data contain key information about the chemical environment of the material through so-called 'chemical shifts' recorded in the binding energy of core electron orbitals. These chemical shifts, however, are extremely difficult to assign, and quantum chemical simulations offer the ideal tool to interpret XPS spectra. However, high-fidelity simulations of large systems are often prohibitively expensive, which motivates the use of machine learning techniques.

The aim of the project is to develop the necessary tools for the evaluation of the energy levels of core electron orbitals, which in turn, will enable the interpretation of photoelectron spectroscopy data. Importantly, the project aims at *making this tooling accessible to experimental chemists from an electronic lab notebook*.

We aim at

- Developing an XPS application for the [cheminfo ELN](#) consisting of reusable JavaScript/TypeScript packages for
 - Parsing and processing of experimental XPS data
 - Spectral fitting
- Python routines
 - Reference database curation and development of lookup and spectral matching protocols
 - Development of machine learning pipelines for fingerprinting, spectral assignment and deconvolution
- Collaboration with the [THEOS group at EPFL](#) for the development of [AiiDA](#) apps for the simulation of XPS spectra and the integration with the cheminfo ELN.

This job opening provides the opportunity to join an exciting and very driven international team at the forefront of research in the field of materials discovery and design. The candidates will join the scientific group at EPFL, and will be working within a team of 10+ PhD students, postdocs, and software specialists with diverse backgrounds (physicists, chemists, materials scientists, computer scientists). They will also be collaborating with groups around the world (at universities, research institutes and companies).

SELECTION CRITERIA

REQUIREMENTS

- Experience with web frontend technologies (HTML, CSS, JavaScript, TypeScript), web/UI frameworks (such as React)
- Strong Python programming skills (including experience with the Jupyter stack)
- Passion for making software tools open and available to a broad audience of users and researchers
- Management of large codes/projects in a team (version control systems, issue trackers, unit testing, continuous integration and other good software practices)
- Experience with REST API (backend) development

Other desirable (but optional) skills:

- Experience in scientific software development
- Experience in running materials simulations on HPC systems
- Experience with software to manage high-throughput runs of simulations
- Experience with Docker and with cloud services – e.g. Amazon AWS, Google Cloud Platform, Microsoft Azure, or OpenStack

Outstanding candidates are sought with a PhD in the physical sciences (e.g. physics, chemistry or materials science/engineering), or comparable skills and experience. Candidates are expected to show excellent work ethics and to feel at home working in teams.

FUNDING AND WORK ENVIRONMENT

The workplace is [EPFL - Valais Wallis \(Sion\)](#).



The contract is renewable every year (as required by EPFL) for up to 4 years upon mutual satisfaction and availability of funding; *current funding is for 12 month*.

APPLICATIONS

Candidates should submit two PDF documents: 1) a full CV, including contacts for at least two references and 2) a letter of intent. The documents should be emailed to kevin.jablonka@epfl.ch, berend.smit@epfl.ch, mounir.mensi@epfl.ch (a single email simultaneously to all, not three separate emails) with the exact text “XPS platform postdoc/software engineer position” in the subject line. Shortlisted candidates will be contacted individually for initial interviews over Zoom video conferencing. For best consideration, applications should be submitted by June 15, 2022; the positions will remain open until suitable candidates have been found.