Doctoral Research Position
"Spectroscopy and quantification of lithium by x-ray microanalysis"

***Employer** : CNRS (French National Center for Scientific Research)*
***Location** : Paris, France*
***Discipline, keywords** : Physical Sciences, X-ray spectroscopy and spectrometry, Electron-matter interaction, Lithium, Electron microprobe, Quantification, Li-bearing minerals*

***Position type** : Full Time, 36 months*
***Job type** : PhD student position*
***Starting date**: October or November 2021*
***Organization type** : Academic*
***Doctoral School:** ED388, Chimie Physique et de Chimie Analytique de Paris Centre*

French ANR (National Agency for Research) committee funds projects that highlight originality, risk-taking and added value for the society. Within this framework, the SQLX project "Spectroscopy and quantification of lithium by X-ray microanalysis", opens a position for PhD student in physics, chemistry with some aspects of geology. This research will be a collaboration between Chimie Physique – Matière et Rayonnement laboratory, Universe Sciences Observatory *Ecce Terra* – Service Camparis, Institut des Sciences de la Terre de Paris (ISTeP), IPGP and CEA-LIST-LNHB, all located in Paris and Ile de France.

We are seeking a candidate with strong skills in physics and chemistry applied to element characterization and quantification. A knowledge of laboratory experience, modeling and electron-matter interactions together with a good practice of spectroscopy, is strongly recommended. The aim of the project is focused on the detection and quantification of lithium through wavelength dispersive X-ray spectroscopy and relies on various tasks.

First, a periodic multilayer designed to disperse the Li K radiation will be implemented on the spectrometer of a standard electron microprobe. This multilayer has already been characterized and results show that this dispersive element is suitable for spectroscopy. This will allow the student to become familiar with this particular spectral range by analyzing reference samples with a spectral resolution of the order of 3 eV.

The second task consists in the implementation and commissioning of a spectrometer working at high spectral resolution, 0.7 eV in Li K range owing to the use of a reflection Fresnel zone plate, on the electron microprobe. With such a spectral resolution, the chemical state of the lithium atoms will be determined from the analysis of the shape of the Li K emission band.

The third task will consist in developing an original model for the quantification of lithium in solids, based on the intensity measurement of the Li X-ray emission band. Since quantification cannot rely on an intensity measurement at a single energy and on a single x-ray attenuation coefficient, emission and absorption spectra will be calculated. For this purpose, *ab initio* calculations of occupied and unoccupied densities will be necessary as well as a critical evaluation of the fundamental parameters, attenuation coefficients and fluorescence yields. This will lead to an elementary quantification model which will be tested first on reference samples and then validated on Li-bearing minerals.

Once the protocol of lithium quantification will be validated, lithium analysis will be performed on natural Li-bearing minerals from various rocks sampled during a field campaign. The study will focus on minerals from pegmatite ores, which constitute one of the major lithium resources on earth. The aim is to identify Li-carriers, potential reactions among these minerals and the processes of lithium mobility and concentration in rocks, in order to better understand the formation of Li-bearing ores and thus anticipate their exploitation potential. Electrodes of Li batteries will be also studied.

Successful candidate will engage with research teams on different labs on issues related to implementation and use of new multilayer mirror and spectrometer, high-level analytical challenges, definition of absorption coefficient and matrix effect. He or she will also be expected to develop new quantification models including partition coefficient and matrix effects correction to determine Li concentration in synthetic or natural solid samples.

REQUIRED QUALIFICATIONS

- Master 2 in physics or chemistry or material sciences with emphasis on X-ray spectrometry research and application in quantification
- Skills in electron-matter interaction, (x-ray) spectrometry
- Passion for multidisciplinary research
- Excellent command of English
- Excellent interpersonal skills and high level of professionalism and tact in interacting with a diverse population of academic collaborators.

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