Postdoctoral Position (12 months, renewable)

Ab initio Simulation of XAS Spectra
New Tool for Energy Materials

Location: ICGM (Institut Charles GERHARDT, Montpellier), www.icgm.fr
Funded by: RS2E (http://www.energie-rs2e.com/en)
Supervisors: Marie-Liesse Doublet (ICGM) & Antonella Iadecola (SOLEIL synchrotron)

Description

Li/Na-rich layered transition metal oxides (LLTMO) are being at the heart of research in the field of **electrochemical energy storage** due to their high energy density. However, they undergo electronic and structural transitions that plague their commercialization. From a theoretical point of view, no clear consensus has yet been reached on the driving force of these transitions, making their control still far. Part of the problem arises from the well-known weakness of **DFT methods** to accurately reproduce the electronic structure of **strongly correlated materials**, and to be predictive on the M-O charge transfer mechanism which is the leading parameter governing the electrochemical response of these materials. In order to fill this gap, **X-ray absorption spectroscopy** (XAS) is the technique of choice to access the electronic as well as the local structure evolution of LLTMO upon cycling. A database made of a large amount of soft and hard XAS spectra for various LLTMOs is already available. This opens new opportunity (i) to benchmark various DFT methods in their ability to reproduce XAS spectra (ii) to check their transferability and (iii) to establish a consensual rationalization of the mechanism(s) underlying the electrochemical performance of LLTMOs as candidates for the future generation of Li/Na-ion batteries. The candidate will benefit of the synergy between the theory group of the RS2E network and the synchrotron SOLEIL.

Requirements:

- Ph.D. in physics, chemistry, materials sciences or related fields.
- Knowledge of ab initio DFT methods
- Experience with theoretical analysis of x-ray absorption spectroscopy
- Basic knowledge in electrochemistry desirable

How to apply?

> Applicants should include a cover letter, a brief summary of accomplishments/interests, a curriculum vitae, a list of publications, and names of 2-3 references. Please send applications to Marie-Liesse.Doublet@umontpellier.fr and antonella.iadecola@synchrotron-soleil.fr

Keywords: DFT calculations – Transition metal oxides – XAS spectroscopy