



Post-doctoral position (12 + 12 months) Joint Project CEA-INAC, CEA-LITEN and ILL, Grenoble, France



Development of *in situ/operando* characterization of advanced lithium-(ion) batteries by neutron scattering techniques

A 12+12 months post-doctoral position is offered in the framework of a long-term project between the CEA and the ILL dedicated to the in-depth study of new electrodes and electrolytes for Li-ion and post-Li ion batteries. This project aims at providing real-time quantification and visualisation of the electrochemical mechanisms at the microscopic level over large time and space scales, by means of *in situ* and *operando* neutron scattering experiments.

Context

Due to the great success of lithium-ion batteries for portable electronic devices, they are nowadays also becoming increasingly important for large-scale applications like electric vehicles. Their widespread implementation, however, is still hampered by several issues as specific energy, power density, durability and safety. The development of safer, more efficient and durable batteries, calls for the design of new nanostructured electrodes and innovative electrolytes to overcome the actual limitations (instability, inflammability, leakage problems, interfacial compatibility, ageing, etc...).

The CEA is a major player in the field of materials synthesis, characterization, design and testing in real devices. Promising approaches include new high energy electrodes (as Li-rich and Silicon nanoparticle-based materials) and novel non-aqueous electrolytes. Understanding the functional properties of these new materials is of paramount importance to improve the performances, and non-intrusive studies of the real-time behavior of batteries are important to characterize and improve the systems.

In situ operando diffraction techniques have been proven to be tools of choices [1,2] to follow the structural modifications of electrodes upon charge/discharge cycling. Yet, the overall behaviour of the battery is also highly conditioned by the electrolyte properties and the electrode/electrolyte interface [3]. The present project aims at a multi-scale multi-technique investigation of the different components of the battery, using neutron scattering performed at the world-class reactor at Institut Laue Langevin. Neutrons are highly sensitive to Lithium and can provide valuable information on Li environment and dynamics. The high neutron flux available at ILL is needed to obtain high quality data and reasonable time resolution.

Objective

We propose to combine state-of-the art neutron diffraction studies, taking advantage of the available electrochemical cell developed at ILL in the framework of an on-going thesis [4], with “soft matter” techniques as SANS/GISANS for structural studies of nanoparticles-based materials and nanostructured electrolytes. This requires the development of ad hoc battery

cells for transmission and grazing incidence geometries. For the most promising electrode/electrolyte couple, QENS experiments could be envisaged to get insights into the molecular mechanism of Lithium diffusion in the materials.

Hosting Teams

The CEA-LITEN team is expert in the conception and implementation of new materials for energy storage. The CEA-INAC team has a renowned activity in multi-scale characterization of the structure/transport interplay of nanostructured materials for energy, including a long-standing experience in operando scattering experiments on fuel cells. A long term visitor status will be provided to the post-doc at the ILL where work will be carried out within the Partnership for Soft Condensed Matter initiative. World leading neutron instrumentation, support facilities, software and instrument experts will be made available and stays at the ILL over short periods of time are foreseen.

Candidate profile

The post doctorate fellow will be in charge of designing/testing the battery cells for neutron experiments (SANS/GISANS/QENS), performing the neutron experiments, analyzing and interpreting the data. He will interact with physicists and chemists of two laboratories of CEA (LITEN and INAC), and with ILL scientists. The candidate must have an excellent knowledge of neutron scattering techniques. As the proposed experimental plan is ambitious and relies on the complementary use of different spectrometers, an advanced experience in diffraction (Rietveld refinements) and/or (GI)SANS and/or QENS is required. Scientific backgrounds in soft matter and/or electrochemistry would be appreciated. Good communication skills will be important to allow the synergy between the various actors involved in the project.

Application: Please join a CV, a cover letter and two recommendation letters.

Contacts

Dr. Hakima MENDIL-JAKANI
CEA/Grenoble, DSM/INAC/SPrAM
Phone: 33(0)4.38.78.91.71
E-mail: hakima.mendil-jakani@cea.fr

Dr. Jean-François COLIN
CEA/Grenoble, DRT/LITEN/DEHT
Phone : 33(0)4.38.78.34.91
E-mail : jean-francois.colin@cea.fr

References

- [1] L. Simonin, J.-F. Colin, V. Ranieri, E. Canevet, J.-F. Martin, C. Bourbon, C. Baetz, P. Strobel, L. Daniel, and S. Patoux. In situ investigations on a li-rich mn-ni layered oxide for li-ion battery. *J. Mater. Chem.*, **22**, 11316–11322, 2012.
- [2] S. Walus, C. Barchasz, J.-F. Colin, J.-F. Martin, E. Elkaim, J.-C. Lepretre, and F. Allouin. New insight into working mechanism of lithium/sulfur batteries: in situ and operando x-ray diffraction characterization. *Chem. Commun.*, **49**:7899–7901, 2013.
- [3] Vetter, J., *Power Sources*, **147**, 269, 2005
- [4] Bianchini, M.; Leriche, J. B.; Laborier, J.-L.; Gendrin, L.; Suard, E.; Croguennec, L. & Masquelier, C. A New Null Matrix Electrochemical Cell for Rietveld Refinements of In-Situ or Operando Neutron Powder Diffraction Data, *Journal of The Electrochemical Society*, **160**, A2176-A2183, 2013