PhD position (3 Years)
A joint CEA / ILL / ESRF project
Grenoble, France - Start March-April 2020

Characterization of all-solid-state batteries using neutron and synchrotron facilities

A 3 years PhD position is offered in the framework of a collaboration between CEA, ILL and ESRF at Grenoble, France, dedicated to the characterization of all solid state batteries using hybrid (polymer-inorganic) **batteries by means of post-mortem and operando scattering and imaging methods**.

Context. The development of solid-state batteries based, for example, on solid electrolytes in replacement of state-of-the art liquid electrolytes, is one of the major challenges to improve the performance and safety of Li-ion batteries for applications in electric mobility and stationary energy storage. The use of non-flammable solid electrolytes is expected to avoid explosions/fire during operation by limiting dendritic growth of Li and reducing leakage. Moreover, advanced electrodes such as lithium metal anodes or high voltage cathodes could be envisaged, yielding improvements in terms of electrochemical stability and volume/mass energy density. To date, there are two main solid electrolyte families:

- Inorganic ionic conductors, i.e. ceramics or glasses. They possess excellent ionic conductivity (up to 10-3 S/cm), good chemical and electrochemical stability and mechanical properties (against dendrites growth). However, these materials are fragile, costly, very sensitive to volume changes and not easily processable.
- Ionic polymers: their main advantages are the ease of processability, low cost and versatility of tunable structures. The main drawback is their insufficient conductivity at room temperature (<10-4 S/cm), as well as limited electrochemical stability at high potential. State-of-the art materials are PEO-based (poly-ethylene-oxide) electrolytes, which require high temperature (80°C) and the use of solvent with a limited transport number of ~ 0.3-0.4.

In this context, **hybrid electrolytes** (combining typically a polymer and a ceramic) are highly appealing materials as they could combine the best properties of organic/inorganic phases, assuring excellent performance (safety, power and energy density) at room temperature and design/process compatibility with low cost industrialisation. The development of these hybrid electrolytes is highly challenging and ambitious as different complex materials need to be mixed and optimised. CEA is launching **a high priority research program** on this topic, supported by UMICORE as an industrial partner strongly involved in the development of new cathode materials adapted to solid-state assembly.

Objectives. The objectives of the PhD student will be the **in depth characterisation of the structure and properties of hybrid electrolytes, including local/nanoscale organisation, organic-inorganic interfaces and electrolyte-electrode interfaces**. The studies will use materials already available at CEA and novel cathodes from UMICORE, as well as new material under development. The student will employ **cutting-edge neutron and synchrotron techniques**, to characterise the hybrid materials both ex situ and operando in devices and propose potential optimisation to the systems. Mixing polymers and ceramics will result in materials of different properties and characteristics depending on the choice of the individual components (molecular architecture of polymers, aspect ratio of particles and crystal structure of inorganic phase), the composition ratio of organic/inorganic mixture, the interfacial interactions and the elaboration process. One main issue is to understand the relation between the hybrid local and nanoscale organisation and the efficiency of ion paths through the various phases and related interfaces. In this regard, ESRF X-ray and ILL neutron techniques are highly relevant tools in terms of core technology challenges (nanostructures and their evolution during the lithiation process, phase transitions, porosity, aging processes, dendritic growth, etc) – providing a holistic view (multimodal, multi-scale). The key techniques to be exploited would be small angle scattering (SAXS and SANS), combined SAXS/WAXS, microbeam SAXS/WAXS (2D mapping), scattering tomography (3D), neutron imaging and nanotomography (ultimate resolution) techniques. In this regard, the opetimzation of dedicated battery cells will be a challenge, as well as the integrated analysis of bug data using optimized (reconstruction/treatment) algorithms.

Hosting Teams. The student would be hired by CEA, with financial support and co-supervision provided by ESRF and ILL. The student would be registered at UGA. CEA is a major player in the field of materials synthesis, characterization, design and testing in real devices in the field of energy conversion and storage. CEA has accumulated knowledge of organic (polymers in salt, polycarbonates, single-ion ionic liquid polymers) and inorganic (LLZO-based) materials over last two years. The objectives are now to perform systematic in depth testing/characterisation under real device conditions, and with an industrial partner on board. To this end, two PhD students (one already started in Jan 2019, focused on materials process and electrochemistry) will work in tandem with the science and technology team at CEA, with UMICORE and exploiting the ESRF and ILL characterisation facilities and skills.
Academic supervisor: Sandrine Lyonnard (CEA, Habilitation in Physics, ED-PHYS at UGA), soft matter physicist specialized in neutron and x-rays studies applied to nanomaterials for energy applications; **Co-supervisor and responsible at ESRF:** Jakub Drnec (ID3) and Manfred Burghammer (ID13) **; Co-supervisor and responsible at ILL:** Lionel Porcar(D22) and Duncan Atkins (D50) **; CEA LITEN science team:** Lionel Picard (organic chemist), Celine Barchasz (battery specialist), Vasily Tarnopolskiy (inorganic chemist) – all battery experts.

Time schedule with milestones (year 1, year 2, year 3)
Year 1: Structural and functional characterisation of individual components. Preparations for ESRF and ILL experiments (lab-based X-ray characterisation, TEM, NMR, design and testing of adapted operando cells).
Year 2: Neutron and synchrotron X-ray experiments to evaluate the hybrid structure ex situ in function of relevant chemical/electrochemical parameters. Investigation of electrolyte/electrode interfaces.
Year 3: Operando neutron and synchrotron experiments performed on solid state cells assembled with best performing hybrid materials and novel cathodes. Focus on lithiation mechanisms, structural aging, dendrite growth and device stability/performance.

Candidate profile:
The PhD student will be in charge of characterizing the physical properties of the newly developed electrolytes by means of neutron/X-rays scattering techniques. He/she will design battery cells and perform the scattering experiments using X-rays lab-spectrometers or the world-class Large Scale facilities (ILL,ESRF), and analyse/interpret the data. He will interact with the physicists/chemists/electrochemists of the CEA (CEA-IRIG and LITEN), the industrial partner, and the synchrotron/neutron experts. The candidate should be a physicist specialized in scattering techniques, and, possibly, data modeling (capabilities to develop/code specific data treatment programs and handle fitting of data batches would be highly appreciated). Scientific backgrounds in nanomaterials as well as interest for battery research would be an excellent basis. Good communication skills will be also 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. Applications until the 10th of September 2019.

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