Type of position: PhD thesis

Title: Digital twins for lifetime enhancement of sodium ion and solid-state battery cells

Context: Sodium ion and solid-state batteries are among the most interesting post-lithium technologies for electrochemical energy storage. In the case of sodium ion battery (SIB) cells, electrodes are composites made of active material, carbon additive and binder, while in the case of solid-state battery (SSB) cells are made of active material, carbon additive, binder and a solid (polymeric and/or ceramic) electrolyte. The performance and durability of these devices strongly depend on the electrode microstructure, *i.e.* on the way the materials are spatially organized within the electrode volume. This spatial organization imply different types of interfaces between the materials, leading to different electrochemical, transport and mechanical limitations. The performance and durability of these cells also depend on the (discharge-charge) cycling conditions which might trigger (electro-)chemical and mechanical degradation mechanisms leading to capacity fade. In the state of the art, the optimization of the cycling conditions of SIBs and SSBs is made by trial and error or design of experiments approaches, which are inefficient in terms of cost and time.

Objectives: We are offering a PhD position, in the context of the BATMAN project (funded through the "PEPR Batteries" Research Program), aiming at developing, validating and demonstrating a digital twin of the function of SIB and SSB cells. Such a digital twin will be able to predict the impact of operating conditions conditions (*e.g.* C-rate, voltage window, temperature) on performance indicators (*e.g.* capacity fade, mechanical failures in the SSB case) at the cell level. Such digital twin will be supported by machine learning models informed with data generated by computational simulations of cell operation based on reduced-order physics-based models and 3D-resolved models using the electrode microstructures generated by manufacturing simulations carried out by another PhD student. The latter physics-based models will account for chemical degradation aspects and will be used to simulate battery behavior from several cycles to full lifetime. Bayesian Optimization will be used on top of the machine learning models, in order to optimize the cycling conditions to enhance lifetime upon charge-discharge cycling. The obtained results will be compared to experimental characterizations carried out in other PEPR projects.

Candidate skills: physical-chemistry or electrochemical engineering, computational modeling, programming (*e.g.* Python, Matlab, Comsol Multiphysics), dynamism, autonomy, team spirit, excellent level of English both spoken and written.

Starting date: as soon as possible.

Place of work: Laboratoire de Réactivité et Chimie des Solides -LRCS- (UMR CNRS 7314), Université de Picardie Jules Verne – 15, rue Baudelocque, 80039 Amiens Cedex, France. The candidate will perform regular visits to IFPEN , rond-point de l'échangeur de Solaize, BP 3, 69360, Solaize, France.

Supervisors: Prof. Alejandro A. Franco (LRCS), Martin Petit (IFPEN).

Please send your CV and motivation letter to: alejandro.franco@u-picardie.fr and martin.petit@ifpen.fr