Type of position: PhD thesis

Title: Digital twins for the manufacturing optimization of sodium ion and solid-state batteries

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 and made of active material, carbon additive, binder and a solid (polymeric 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 electrode microstructure in SIBs and SSBs is strongly determined by its manufacturing process. SIB electrodes are usually made through a wet process where slurries are prepared, casted on current collectors, dried and finally calendered to enhance their electronic conductivity. For SSB electrodes, multiple manufacturing approaches are being considered, but the wet process is probably the most scalable one in view of their similarities with Lithium Ion Batteries (LIBs) electrode manufacturing. In the state of the art, the optimization of the manufacturing process 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), with the goal of developing, validating and demonstrating a digital twin of the manufacturing process of SIB and SSB electrodes. Such digital twin will allow to assess and optimize the correlations between electrode manufacturing parameters (*e.g.* formulation, solvent drying rate, calendering pressure) & properties (*e.g.* materials interfaces), for both SIBs and SSBs. Such digital twin will be supported on a physics-based process modeling framework combining different simulation methods (coarse-grained particle dynamics, discrete element method, Lattice Boltzmann method) and machine learning models, that will be adapted from the ARTISTIC modeling workflow previously developed for LIBs (www.erc-artistic.eu). This framework will be supplemented by virtual material design approaches proposed in the plug im platform (www.plugim.fr) such as aggregation-controlled microstructure model or FFT-homogenization. The digital twin will be able to predict the influence of wet manufacturing parameters on electrode microstructures in 3D. Based on realistic microstructure generation, numerical characterizations will assess the textural properties of the resulting electrode microstructures, such as pore size distributions, surface area of contact between different materials or tortuosity. Stochastic generation will be also used to augment the databases produced by the physics-based and machine-learning based models. The resulting computational workflow will be coupled to a Bayesian optimization algorithm which will allow to perform inverse design of manufacturing parameters to achieve desired electrodes properties. The obtained results will be compared to experimental characterizations carried out in other PEPR projects.

Candidate skills: physical-chemistry or process engineering, computational modeling, programming (*e.g.* Python, LAMMPS), 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 IFP Energies nouvelles, rond-point de l'échangeur de Solaize, BP 3, 69360, Solaize, France.

Supervisors: Prof. Alejandro A. Franco (LRCS), Dr. Maxime Moreaud (IFPEN).

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