Type of position: PhD thesis

Title: Computational modeling of lithium ion battery electrode manufacturing

Context: The needed massive deployment of lithium ion batteries (LIBs), in particular to satisfy the demand from the Electric Vehicle sector, encourage battery manufacturers to multiply the number of giga-factories to reduce the cost of production. Such a production consists of a complex process involving multiple steps, such as the slurry preparation, its coating, drying, calendering, electrolyte filling and formation. The choice of the manufacturing parameters along the process strongly impact the overall LIB cell performance. However, the optimization of the manufacturing parameters to obtain the desired characteristics of LIB cells is heavily based on a forward "trial and error" approach. This approach is inefficient in terms of time and cost due to the infinite number of possibilities for adjusting the manufacturing parameters. The use of digital tools based on numerical simulation and artificial intelligence is essential to accelerate the manufacturing process optimization.

Objectives: We propose here a PhD thesis to work on the computational modeling of the manufacturing process of LIB electrodes. The intended computational modeling will be physics-based and will be supported on Coarse Grained Molecular and Particle Dynamics, as well as on the Discrete Element Method, by using software like LAMMPS. The work will consist at first adapting the pre-existing ARTISTIC manufacturing simulation framework developed by Prof. Alejandro A. Franco's group at Université de Picardie Jules Verne (LRCS) to the materials chemistries undertaken by ARKEMA. The candidate will work on the utilization of these models to investigate the influence of manufacturing parameters (e.g. formulation, drying rate, calendering degree) on the 3D-resolved electrodes microstructures. Associated electrode properties will be assessed such as porosity, tortuosity factor, conductivity, energy and power densities using a wide diversity of ARTISTIC scripts. The modeling results will be confronted to the experimental data generated by ARKEMA, which will allow the calibration and validation of these models.

Candidate skills: physical-chemistry or process engineering, computational modeling, dynamism, autonomy, team spirit, excellent level of English both spoken and written.

Starting date: September-October 2023.

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 ARKEMA – Centre de Recherche Rhone-Alpes.

Supervisors: Prof. Alejandro A. Franco (LRCS), Mathilde Koch (ARKEMA).

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