Master thesis proposal

February 11th – August 10th 2019

Title of the research topic	**Investigation of battery manufacturing parameter interdependencies (ERC-funded ARTISTIC Project)**
Laboratory or Company	**Laboratoire de Réactivité et Chimie des Solides (LRCS)**
Laboratory Director	**Mathieu Morcrette**
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Scientific Project: The general goal of the ERC-funded ARTISTIC project is the development of a multiscale modelling platform that rationalizes the formulation and fabrication process of Li-ion battery (LIB) composite electrodes (made of active material particles, carbon additive particles and binder) and the effect of the variables of each step of the manufacturing process in the architecture and electrochemical operation of them. A predictive open access computational platform is being developed through the combination of discrete particle and continuum mathematical models within a workflow that integrates the individual models and mimics the different steps along the electrode fabrication process, including the slurry preparation, electrode film drying and calendaring. This platform is supported by intensive experimental characterization which unravels the existing complex interdependencies between the fabrication process steps: variation of a single process parameter can cause a variety of other parameters to change. For instance, variation in the slurry composition will affect the viscosity, which will in turn impact the choice of parameters for the electrode film drying and the calendering conditions. Many of these interdependencies are currently known qualitatively or in an isolated way.

In order to rationalize such parameter interdependencies and for the sake of the ARTISTIC models' parameterization, it is crucial to organize the experimental and simulation data within an appropriate workflow format. The objective of this MSc thesis is to develop an integrative dataset framework, with uniform format for experimental and modeling results, and which clearly sets out the fabrication steps inter-relationships; stating the inputs, outputs and inter-connections between each of them, as well as the metadata. Such a dataset will need to interface Excel files with a master script (e.g. coded in Python) which will ease the automatic reading and the search of data. The script will permit the quantification of uncertainties propagations between steps, stablishing statistical correlation tests needed for asserting relationships between the fabrication steps parameters and the final LIB electrochemical performance. The main outcome of this project will be a standardized dataset for the ARTISTIC project which 1) will ease the parameterization of the force fields in the Coarse Grained Molecular Dynamics simulations used to simulate the electrode film formation; and 2) will be used for training machine learning algorithms aiming to predict the impact of fabrication parameters on the LIB electrode properties.

This MSc. project will be carried out in close collaboration with the Laboratoire Amiénois de Mathématiques Fondamentales et Appliquées (LAMFA), the mathematics laboratory of our University (Professors Jean-Paul Chehab, Youcef Mammeri and Mark Asch). Candidates should be MSc. students (M2) or engineer students, with excellent background in statistics, applied mathematics and programming. Some knowledge in machine learning techniques will be highly appreciated. They should be open-minded, dynamic and show a strong motivation.

Techniques used:

- Statistical analysis, data analytics;
- Uncertainty Quantification methodologies;
- Python programming language.

Recent publications related to the topic :
1. A. C. Ngandjong, A. Rucci, M. Maiza, G. Shukla, J. Vazquez-Arenas, A. A. Franco; *The Journal of Physical Chemistry Letters* **2017** *8* (23) 5966-5972.
2. M. Thomitzek, O. Schmidt, F. Röder, U. Krewer, C. Herrmann, S. Thiede; *Procedia CIRP* **2018** *72* 346-351.
3. A. Chernatynskiy, S. R. Phillpot, R. LeSar; *Annual Review of Materials Research*, **2013** *43* 157-182.
4. K.K. Bejagam, S. Singh, Y. An, S.A. Deshmukh; *The Journal of Physical Chemistry Letters* **2018** *9* 4667-4672.