ERC Consolidator Project “ARTISTIC”

Opening PhD and postdoctoral positions

Several PhD and postdoctoral positions will become available within the framework of the ERC Consolidator project “Advanced and Reusable Theory for the In Silico optimization of composite electrode fabrication processes for rechargeable battery Technologies with Innovative Chemistries” (ARTISTIC) lead by Prof. Alejandro A. Franco at the Laboratoire de Réactivité et Chimie des Solides (UMR CNRS 7314, Université de Picardie Jules Verne, Amiens, France). The objective of this project is to develop a computational platform for the prediction of optimal fabrication processes and electrochemical performance of lithium ion battery electrodes. The recruited PhD students and postdocs will be outstanding individuals, highly dynamic, creative and motivated to join an international project team of excellence addressing highly challenging research tasks coupling computational modeling with experimental activities.

PhD and postdoctoral candidates on the topic of modeling are required to have:

- Excellent skills in theoretical physics, and physical-chemistry and/or electrochemistry. Experience in the battery field will be a plus;
- Excellent skills and/or deep experience in programming (*e.g.* Python, CUDA) and in using scientific calculation techniques (*e.g.* coarse grained molecular dynamics, kinetic Monte Carlo, lattice Boltzmann, continuum modeling) and software (*e.g.* Matlab, COMSOL Multiphysics, LAMMPS, GROMACS);
- Skills on parallel and GPU computing will be a plus.

Candidates having experience only on electronic calculations (Density Functional Theory or similar) will not be considered.

PhD and postdoctoral candidates on the experimental activities are required to have:

- Excellent skills in physics, chemistry and electrochemistry. Experience in the battery field will be a plus;
- Excellent skills and/or deep experience in process and/or electrochemical engineering, materials characterization (*e.g.* viscosimetry, porosimetry, BET, SEM, TEM) and electrochemistry techniques (*e.g.* electrochemical impedance spectroscopy).

“Mixed profiles” (having both modeling and experimental skills) will be particularly studied.

All candidates are required to have:

- Excellent organizational and time-management skills;
- Ability to communicate results clearly and succinctly;
- Ability to work as a team member and to work independently;
- Excellent level of English, both written and spoken;

- Candidates for postdoctoral positions should have a recently obtained PhD diploma (not older than 1 year at the application date) and a significant track record of publications.

The recruited PhD students and postdoctoral researchers will

- Carry out research about the fabrication process of battery electrodes, and its link to the electrochemical performance;
- Monitor the work plan of her/his individual research project and make sure that milestones are achieved and tasks are finalized in a timely manner;
- Actively participate in research meetings with the other ERC team members;
- Take part in the research meetings, seminars, etc. at the LRCS laboratory, RS2E and ALISTORE ERI networks;
- Assist in the supervision of MSc. Students.

Time frame and location:

Some of these positions will start at the beginning of the project, others later.

PhD positions are for 3 years, and postdoctoral positions are for 1+1 year.

The place of work will be the Laboratoire de Réactivité et Chimie des Solides (UMR CNRS 7314) in Amiens, France.

Application modalities:

Interested individuals are requested to send to Prof. Alejandro A. Franco's email (alejandro.franco@u-picardie.fr) the following materials:

- Detailed CV;
- Copy of the 3 most recent publications (if available);
- Motivation letter specific to the ERC project ARTISTIC (applications with generic motivation letters will not be responded);
- The names and contact details of 4 reference persons, at least from 2 different institutions.

The ARTISTIC Project

The aim of this project is to develop and to demonstrate a novel theoretical framework devoted to rationalizing the formulation of composite electrodes containing next-generation material chemistries for high energy density secondary batteries. The framework will be established through the combination of discrete particle and continuum mathematical models within a multiscale computational workflow integrating the individual models and mimicking the different steps along the electrode fabrication process, including slurry preparation, drying and calendering. Strongly complemented by dedicated experimental characterizations which are devoted to its validation, the goal of this framework is to provide insights about the impacts of material properties and fabrication process parameters on the electrode mesostructures and their corresponding correlation to the resulting electrochemical performance. It targets self-organization mechanisms of material mixtures in slurries by considering the interactions between the active and conductive materials, solvent, binders and dispersants and the relationship between the materials properties such as surface chemistry and wettability. Optimal electrode formulation, fabrication process and the arising electrode mesostructure can then be achieved. Additionally, the framework will be integrated into an online and open access infrastructure, allowing predictive direct and reverse engineering for optimized electrode designs to attain high quality electrochemical performances. Through the demonstration of a multidisciplinary, flexible and transferable framework, this project has tremendous potential to provide insights leading to proposals of new and highly efficient industrial techniques for the fabrication of cheaper and reliable next-generation secondary battery electrodes for a wide spectrum of applications, including Electric Transportation.

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