PhD thesis position on Modeling of Redox Flow Batteries, Amiens, FRANCE https://www.lrcs.u-picardie.fr/	
Topic Title	Computational Modeling of Redox Flow Batteries
Principal Advisor	FRANCO, Alejandro A. alejandro.franco@u-picardie.fr
Co-advisor	
Web Site of Advisor (if applicable)	https://www.u-picardie.fr/erc-artistic/ www.modeling-electrochemistry.com
Date of publication of the offer	September 13, 2019
Deadline for application	October 30, 2019
Date of start of the Project	January 6, 2020 (duration: 3 years)
Description of the Topic	This thesis project focuses on the development of an innovative series of physical models for computer simulation of the electrochemical behavior of redox flow batteries comprising anolytes and catholytes based on organic molecules. The novelty of these models is based on the focused scale (mesoscopic) and the computational approaches used (kinetic Monte Carlo, Dissipative Particle Dynamics, Lattice Boltzmann, continuum ...). These models will effectively describe electrochemical reactions at interfaces, degradation reactions and convective transport mechanisms, while keeping a quasi-molecular dynamics description. They will simulate the electrochemical response of the battery cell according to the operating parameters. The input parameters required for building the models as well as the simulation results will be determined / compared by / with dedicated experimental measurements. The models will integrate a multiscale simulation platform developed in the European project SONAR, funding this thesis, to automatically optimize the chemistries of the anolytes and catholytes used in these batteries. **Context:** The work will take place in the Laboratoire de Réactivité et Chimie des Solides (UMR CNRS 7314), located in the Energy HUB (University of Picardy Jules Verne, Amiens, France). This project is part of the European project "SONAR", which has been recently accepted for funding by the Horizon 2020 research program. This project aims at developing a multi-scale simulation platform allowing to perform automatic screening of the impact of the chemical composition of anolytes and catholytes on the electrochemical response of redox flow batteries.
Skills of the Applicant	Physics or electrochemical engineering or physical chemistry with background in applied mathematics and numerical simulation. Knowledge in programming or experience with scientific computing software. Teamwork. Dynamism. Autonomy. Very good level of written and spoken English.
Contact (s)	alejandro.franco@u-picardie.fr
List of documents to provide	CV + motivation letter + list of references