# Modeling and synthesis of 3D structured-polymer electrolyte to regulate Li dendrite formation during cycling of Li metal battery

## Context

In order to achieve successful electric vehicles, it is crucial to enhance the energy density of batteries. Among the various battery systems, Li metal batteries have emerged as one of the most promising options since it offers the highest theoretical capacity and the lowest negative electrochemical potential. However, the commercialization of Li metal batteries has faced challenges, primarily attributed to the uncontrollable Li dendrite formation during battery cycling. This issue becomes even more critical when applying high voltage for applying the battery to electric vehicle. To address this, significant research has been conducted on polymer electrolytes for Li metal batteries, as they hold the potential to revolutionize the electric vehicle industry. Various 3D structured-polymer electrolytes synthesized through different polymerization methods have exhibited remarkable capabilities in regulating the formation of Li dendrites. Battery life span is longer with 3D structured-polymer electrolyte compared to common liquid electrolyte; it seems promising for future Li metal battery design. Nonetheless, the precise mechanism behind how these 3D structured-polymer electrolytes regulate Li dendrite formation remains unclear.

## Objective

Our primary goal is the understanding of Li dendrite formation at the interface between Li metal and 3D structured-polymer materials. Building upon this knowledge, we aim to design a novel polymer electrolyte that addresses the challenges associated with Li dendrite formation. To achieve our goals, we will employ a combined approach of experimental and theoretical methods. During the project, the Ph.D. candidate will synthesize and characterize the 3D structured polymer electrolyte. In parallel, student will model the polymer electrolyte system by using state-of-art modeling solution. We will train the Ph.D. candidate to allow s/he conduct research independently and become expert of electrochemistry and atomistic level of simulation.

## Requirement of applicant

- We are looking for a motivated candidate with strong knowledge in polymer synthesis and characterization for this thesis. Additionally, candidates with a background in computational chemistry, specifically in performing DFT calculations and MD simulations, as well as experience in electrochemical analysis for battery testing, will be preferred.

- Proficiency in English is essential, as the candidate will be expected to write manuscripts and communicate the research findings in English.

**Contact information:** matthieu.becuwe@u-picardie.fr (LRCS) / junghan.son@renault.com (Renault)

**List of documents required:** CV (not more than 1 page), Motivation letter (not more than 1 page), recommendation letters (Ideally the letters from 2 person, contact details of the reference person should be presented)

**Date of start of the Project:** end of 2023 **Duration:** 36 months

**Location*:** Laboratoire de Réactivité et Chimie des Solides (CNRS UMR 7314) in Amiens, France // Technocentre (TCR) Renault, in Guyancourt.

*Most of research activities will be performed in Amiens, you will visit TCR around once per two months.