## « Unravelling the Spectroscopic Signatures of Solid-Electrolyte Interfaces using Theoretical Chemistry Methods »

**A PhD position** is available in the Theoretical Chemistry Lab (http://www.unamur.be/en/sci/chemistry/lct ) of the University of Namur and the newly-established Namur Institute of Structured Matter (http://nism.unamur.be ).

**Details and frame of the project and PhD Thesis.** Within a multidisciplinary framework involving the KU Leuven, UCLouvain, UBonn, and UNamur the ECOBAT's project aims to provide new knowledge and materials to build, test, and compare the performance metrics of different s-block elements in Metal-Anode Batteries (MABs) and identifying the common elements governing the bulk, interface, and solvation properties of s-block MABs. More specifically, ECOBAT aims at understanding the effect of the solvent and salt anion on reversible metal deposition and metal-ion intercalation in MABs using a single type of cathode materials and at unraveling the relationship between the first coordination sphere and the electrochemical properties of the metal ions in organic media.

The proposed PhD project targets the understanding and prediction of the Solid-Electrolyte Interface (SEI) growth models by using theoretical chemistry methods. This encompasses *e.g.* i) sampling the configuration space to identify important structures, ii) evaluating electrolytes-solvent binding energies, and iii) simulating their spectroscopic signatures to be compared to experimental data. Several levels of approximation are foreseen i) from DFT calculations on finite size systems to PBCs calculations on slabs and ii) from classical to *ab initio* MD simulations.

**Offer**. Following the legal scale in Belgium, the grant will amount to about 2350 € per month. The candidate will be working in the research group of Prof. Benoît CHAMPAGNE and use computational facilities provided by the HPC consortium of the Fédération Wallonie-Bruxelles, including those of the Scientific Computing Platform of our University. Her/his secondment will be carried out in the group of Prof. Barbara KIRCHNER (https://www.chemie.uni-bonn.de/kirchner/de ).

**Requirements**. Highly motivated candidates with i) a Master in Chemistry/Physics or Engineering Sciences or in related areas (Master recently obtained, no more than 4 years), ii) with an expertise in theoretical/quantum chemistry and/or in numerical simulations in chemistry/physics of materials, iii) an expertise in multi-scale simulation methods is an asset, iv) abilities to communicate (sufficient level in English combined with good pedagogical skills) and to work in a team, including theoreticians and experimentalists, while v) an expertise in scientific programming (fortran, C++, python, ...) in view of writing new codes and of modifying existing ones is an asset.

**How to apply**. Interested candidates should send their curriculum vitae, including their scientific achievements, list of publications, coding skills, and cover letter explaining why they feel being the right person for this position, and a list of, at least 2, contact reference e-mails (**in a single PDF file**) to Prof. Benoît CHAMPAGNE, benoit.champagne@unamur.be. Candidates are advised to apply as early as possible. The selection process will start immediately.