

Molecular modeling of polymer-electrolyte interfaces in hybrid-solid battery applications

PhD position at [IFP Energies nouvelles](#) (IFPEN)

In view of the rapidly increasing demand for electrical energy storage, particularly in the field of transportation, significant research efforts are being undertaken to develop new generations of lithium batteries. Academic and industrial research currently focus on energy density enhancement and battery safety. Lithium-ion batteries are today the most interesting solution to answer the ever-increasing demand for electrochemical energy storage devices. The two main requirements for such systems are a higher gravimetric capacity and an increased safety, both can be addressed using solid electrolytes instead of the liquid ones in the current technology. At present time, three main groups of solid electrolytes exist: polymers, inorganic materials, and hybrid materials (a mixture of an inorganic and an organic phase). Hybrids are promising as they combine the high ionic conductivity of inorganic electrolytes and better mechanical properties and processing of polymers. The research on hybrid electrolytes has uncovered an important challenge: the organic-inorganic interface. In some cases, these interfaces can greatly decrease ionic conductivity and thus hinder battery performance. A better understanding of the chemical, physical and electrochemical properties (conductivity, stability) is crucial to master the development of competitive hybrid electrolytes. This PhD will focus on the understanding of the cohesion, stability, and ion transfer mechanisms at the polymer- inorganic electrolyte of the interface of hybrid electrolytes from an atomistic point of view by using a molecular simulation approach. First realistic models of the interfaces at the atomistic scale will be developed based on preexisting first principles calculations. These results will be used for the development of intermolecular potentials or machine learning potentials that explicitly include polarization to accurately describe the Li transport in bulk electrolytes. Then, the simulations will be extended to solid inorganic electrolyte-polymer model interfaces, to understand the effect of the interface structure on important properties (adhesion forces, ion transport, etc.). The aim will be to develop characterization and modeling techniques of the interface that can be extended to different families of hybrid electrolytes, or even to study unknown phases.

Your Qualifications

You should have a Master's degree in Chemistry, Physical Chemistry or Physics with strong motivation in scientific research and innovation and team collaboration spirit. You have good academic ethics, rigorous scientific attitude and general knowledge in physical chemistry with notions in the following fields: electrochemistry, molecular modeling, programming (Python) & machine learning. Skills in composite materials chemistry or formulation would be a plus. A B2 level in English (CEFR) is compulsory. The starting date will be on the 4th trimester of 2024.

We Offer

The 3-year PhD location will be IFP Energies nouvelles (Rueil-Malmaison, France). Our institution is a leading research institute that is globally recognized for its research, innovation, and scientific value. The doctoral school will be the ED388 "Chimie Physique et Analytique de Paris Centre", with a diploma delivered by "Sorbonne Université". The project will be in collaboration with Professor T. Verstraelen from the [Center for Molecular Modeling](#) at Ghent University (Belgium).

Application procedure

Applications must be submitted to [Dr. Carlos Nieto-Draghi](mailto:carlos.nieto@ifpen.fr) (carlos.nieto@ifpen.fr, ORCID: [0000-0001-5956-9259](https://orcid.org/0000-0001-5956-9259)), [Dr. Manuel Corral-Valero](mailto:manuel.corral-valero@ifpen.fr) (manuel.corral-valero@ifpen.fr) or [Dr. Theodorus de Bruin](mailto:theodorus.de-bruin@ifpen.fr) (theodorus.de-bruin@ifpen.fr), with the following elements: 1) Application (motivation letter stating their research interests), 2) CV, 3) Copy of academic diplomas (MSc), 4) 2 Letters of recommendations.