Molecular Modeling of Inorganic Electrolyte/Organic Polymer Interphases in Hybrid Solid State Batteries

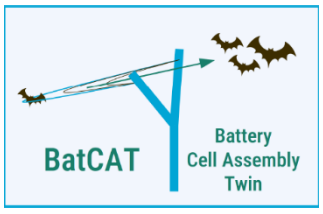
Postdoc position at IFP Energies nouvelles (IFPEN)

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. The use of solid electrolytes improves safety by avoiding the use of solvents and flammable liquid electrolytes. Additionally, in hybrid lithium solid-state batteries (LiSSBs) inorganic solid electrolytes (SE) assure a high electric conductivity, whereas organic polymeric (OP) binders improve mechanical properties. Although the combination of SE with OP is promising, some systems are unstable, which diminishes their potential long-term use. As these are very complex composite materials, little is known about their structure and reactivity.

In this project, we aim at unravelling the structure and reactivity of some SE-OP systems by first principles calculations. The selected postdoc will start to do a bibliographic study that is centred on the surface properties and transport mechanisms in solid electrolytes, with a focus on contributions from molecular modelling AIMD (DFT) simulations and extends the survey on the modelling of in/organic interfaces with machine learning methods. Based on knowledge from both internal and open literature, representative models including electrolyte as well as the polymer/electrolyte interfaces will be constructed and fully analysed with respect to their interaction energies and Li-transport properties using computational techniques.

Your Qualifications

You are under 35 years old, having obtained a PhD no more than 3 years ago in theoretical/computational physics or chemistry. You have strong scientific research and innovation skills and team collaboration spirit. You have good academic ethics, rigorous scientific attitude. Proficiency in software like VASP, CP2K or LAMMPS is highly preferred. You have good programming skills and a good knowledge of Python. Finally, you have excellent communication skills in both spoken and written English. French is not a prerequisite, but a basic knowledge (level A2 or B1) is recommended. Applicants with significant scientific achievements are prioritized. **This postdoc is immediately available,** and it is part of the **European BatCat-101137725 project** and should ideally start at T2/2024.



We Offer

IFP Energies nouvelles is a leading research institute that is globally recognized for its research, innovation and scientific value. We offer a rewarding and challenging job in an international environment, with a gross monthly salary of 3000 €. We strive for excellence in an environment characterized by collegial respect and responsibility. The work is principally carried at Rueil-Malmaison (close to Paris).

Application procedure

Applications must be submitted to Dr. Carlos Nieto-Draghi (carlos.nieto@ifpen.fr), Dr. Manuel Corral-Valero (manuel.corral-valero@ifpen.fr) or Dr. Theodorus de Bruin (theodorus.de-bruin@ifpen.fr).with the following elements:

- Application (motivation letter stating their research interests)
- CV
- Copy of academic diplomas (MSc/PhD)
- 2 Letters of recommendations
- List of publications