## Postdoctoral Position

**Métier ou emploi type**: REME, REFERENS, BIBLIOPHILE

**Position**: Postdoctoral researcher

**Catégorie**, **Corps**: BAP (si ITRF)

Les activités qui composent la fiche de poste sont appelées à évoluer en fonction des connaissances du métier et des nécessités de service.

### About Sorbonne Université

Sorbonne Université was created on January 1st, 2018 from the merger of Paris-Sorbonne and Pierre and Marie Curie (UPMC) universities. As a public institution, it fulfills the public service calling of French higher education, research and innovation. Sorbonne Université is a multidisciplinary and research-intensive university with world-famous origins. Continuing the humanist tradition of the Sorbonne, it is devoted to meeting the scientific challenges of the 21st century and spreading the knowledge created in its laboratories by its research teams and transmitted to its students and to society as a whole. Sorbonne Université’s three faculties in humanities, medicine and science each with the wide-ranging autonomy necessary to conduct its ambitious programs in both research and education. The university’s 53,500 students, 3,400 professor-researchers and 3,600 administrative and technical staff members who help it run every day contribute to a University that is diverse, creative, innovative, and with a global outlook.

### About the Institute of Computational and Data Sciences (ISCD)

**Description**: The Institute of Computing and Data Sciences (ISCD, https://iscd.sorbonne-universite.fr/) is dedicated to exploring and developing the potential of computational and data-driven research and training across science, humanities and medicine at Sorbonne Université. Our research teams develop and use algorithms and visualization methods to solve problems in biology, chemistry, mathematics, computer science, medicine and digital humanities. The ISCD was created more than ten years ago, to support areas where methods and means of addressing challenges transcend disciplines and profoundly transform research.

The candidate will also be integrated in research teams within the PHENIX (PHysicochimie des Electrolytes et Nanosystèmes InterfaciauX) and IMPMC (Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie) laboratories, nearby ISCD. The candidate will therefore be able to interact with researchers specializing in computer science, as well as physical and chemical sciences.

**Location**: Esclangon building, Campus Pierre et Marie Curie, 5 place Jussieu, 75005 Paris

### Description of the Project and its Activities
Description of the Project:

**Scientific background:** Extending the lifetime of aqueous batteries is critical to enable practical applications. It is currently limited by chemical reactions occurring in the electrolyte in uncontrolled ways. Using computer simulations, our aim is to understand how and why these reactions happen. Standard techniques limit us to only a handful of reactions [1]; in addition, recent work [2] showed that the structure of some important aqueous-based electrolytes such as water-in-salts is not correctly captured by simple analytical interatomic potentials. For these reasons, we propose to deploy a machine learning approach to accelerate our simulations. The aim of this project is to achieve a microscopic understanding of aqueous battery ageing – in addition, we could provide guidelines to experimentalists to design electrolytes with improved performances.

**Scientific objectives:** There are two main objectives in this research project. The first one is to implement a machine-learned interatomic potential, trained on ab initio data, able to capture key structural traits of aqueous-based electrolytes. For that purpose, modern message-passing architectures such as the Allegro model [3] will be implemented. The second objective is to study chemical reactions involving the degradation of bistriflimide (TFSI-), such as nucleophilic attacks by hydroxide. Estimates of the free energy profile along reaction coordinates will be obtained with enhanced sampling techniques (metadynamics, umbrella sampling), applied to molecular dynamics data obtained with a machine-learned interatomic potential. Emphasis will be placed on investigating the transferability of such models depending on the training data, when describing chemical reactions. The free energy profiles, intermediate products, and reaction pathways will be compared to results obtained through radiolysis experiments by Sophie Le Caër and her team, at CEA [4].

Finally, the candidate will interact with many researchers from ISCD, PHENIX, and IMPMC; they will be able to collaborate on projects related to the precipitation and crystallization of salt at the interface formed between a liquid electrolyte and a solid electrode, as well as theoretical and numerical developments related to enhanced sampling, collective variables, and coarse-grained models.


Main Activities :
• Molecular dynamics simulations applied to complex materials
• Methodological and code development
• Writing of scientific articles
• Participation in conferences

Supervision : No

Skills and Competences

**General Background:** Chemical physics, statistical mechanics, reactivity

**Skills:** molecular modeling

**Transversal skills:** machine learning, code development

**Other skills:** both working as part of a team and individually

**Other conditions :** /