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SORBONNE UNIVERSITÉ

MINISTÈRE
DE L'ENSEIGNEMENT SUPÉRIEUR
ET DE LA RECHERCHE

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 fulfils 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 be part of the interdisciplinary MAESTRO team, which includes chemists, physicists and mathematicians. The long-term goal of MEASTRO is to **study the properties of materials by stochastic sampling and high-performance computing.** **Location : Esclangon building, Campus Pierre et Marie Curie, 5 place Jussieu, 75005 Paris**
Description of the Project and its Activities

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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. While standard techniques limit us to only a handful of reactions [1], 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: The main objective of this project will be to study two classes of reactions involving the degradation of bistriflimide (TFSI-): nucleophilic attacks by hydroxide, and reactions mediated by electron insertion. Estimates of the free energy profile along reaction coordinates will be obtained with enhanced sampling techniques (metadynamics, umbrella sampling), applied to *ab initio* molecular dynamics simulations accelerated with machine learning. The acceleration will be handled using a surrogate model trained on-the-fly [2]. 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 [3].

Finally, the candidate will be part of the interdisciplinary MAESTRO team, and 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.

[1] A. France-Lanord, F. Pietrucci, A. M. Saitta, J. M. Tarascon, A. Grimaud, A., M. Salanne, *PRX Energy, 1* (1) 013005
[2] R. Jinnouchi, J. Lahnsteiner, F. Karsai, G. Kresse, M. Bodam (2019), *Physical review letters, 122*(22), 225701
[3] Y. Levieux-Souid, J.-F. Martin, P. Moreau, N. Herlin-Boime, S. Le Caër (2022), *Small methods*, 6(10), 2200712

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 : /

* Conformément à l'annexe de l'arrêté du 18 mars 2013 (NOR : MENH1305559A)