Institut des sciences du calcul et des données
SORBONNE UNIVERSITÉ

Job Offer

Job Summary

Title, Job Position	Postdoctoral position: Generalized Langevin equations and stochastic sampling
Research Field	Applied mathematics
Employer	Sorbonne Université Institut des sciences du calcul et des données
Location :	Paris, France
Application Deadline / Timezone	15-02-2020 11:00AM Paris (GMT+01 :00)
Salary	depending on skills and experience
Type of Contract	Temporary (fixed term) 18 months
Job Status	Full-time
Envisaged Starting Date	Between 15 April and 15 June 2020

Hiring Organisation

Organisation

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 University 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 University'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.

Organisation Type

Higher Education Institute

Department

Institut des sciences du calcul et des données, FED 3

The institute of computing and data sciences (ISCD (http://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 use the power of algorithms and visualisation to solve problems in biology, chemistry, mathematics, computer science, medicine, and the digital humanities. Our history of supporting collaboration goes back more than 10 years when the institute was created to support areas where methods and means of approaching challenges spilled over the disciplines. and were profoundly transforming research.

Offer Description

Description

Scientific context. Molecular simulation is the main tool for the prediction of kinetic properties of physico-chemical systems in computational physics and materials science. The most satisfactory framework to describe and understand the dynamics of metastable transitions consists in projecting the high-dimensional trajectory of the system (thousands of Cartesian atomic coordinates) onto a low-dimensional space of collective variables. This dimensional reduction leads to a stochastic differential equation (SDE) – a so-called effective dynamic – which should in general be non-Markovian (generalized Langevin equation).

Scientific environment. The post-doctoral project is part of the new MAESTRO interdisciplinary team, within the Institute for Computing and Data Sciences (ISCD) in Sorbonne Université. By joining forces between mathematicians, physicists and physical chemists, the long-term goal of the team is to investigate materials for energy through stochastic sampling and high-performance computing.

Scientific objectives. The objective of the first phase (2 years) of the project is the development of a systematic approach to construct accurate Langevin models of dynamical processes in complex materials, employing as input data extensive molecular dynamics trajectories. These trajectories are often too short to obtain accurate statistics, and we need a model to compute long time dynamics.

The main challenges to solve in this direction are the development of efficient stochastic optimization, unbiased statistical estimators and variance reduction techniques, as well as the definition of general strategies (e.g. variational principles) to identify optimal collective variables and to tackle non-Markovian memory effects.

The study will primarily focus on simple “toy” models, in order to identify the key steps and overcome the mathematical bottlenecks without being limited by the numerical cost and physical complexity. The results will then be transferred to challenging systems in materials science.

Project PI: A. Marco SAITTA

Postdoc supervisors: Pierre MONMARCHE – Ludovic GOUDENEGE – Fabio PIETRUCCI – Benjamin ROTENBERG

Appointment Term

Eighteen months appointment starting as soon as possible.

Keywords: Generalized Langevin diffusion; colored noise; effective/coarse-grained dynamics; sampling methods; material science; numerical simulation; molecular dynamics

As part of your duties, you may be required to provide internal training related to your business expertise.

Profile Requirements

Required Education Level

Expertise in probability, statistics and stochastic algorithms. Monte-Carlo methods and Bayesian statistics. Stochastic optimization.

Skills / Qualifications

- Applicants must have a recent Ph.D. in Mathematics
- Prior experience and proficiency in numerical algorithms and stochastic optimization
- Applicants should be hard working, analytical and have excellent writing and communication skills necessary to author technical and scientific reports, publications, and deliver scientific presentations, seminars, meetings and/or teaching lectures
- Experience collaborating effectively with a team of scientists of diverse backgrounds

Specific Requirements

- This position involves a significant amount of numerical code development
    - Therefore the candidate will have prior scientific programming experience combined with an enthusiasm for scalable computing.

Required Languages

English

Required Research Experience

PhD/previous postdocs in research-intensive labs, significant publication record

Work Location

Institute

Institut des sciences du calcul et des données
Equipe-projet "*Maestro*" (The **MA**terials for **E**nergy through **ST**ochastic sampling and high pe**R**formance c**O**mputing) – PI: A. Marco SAITTA

Country

France

Location

Sorbonne Université
Campus Pierre et Marie Curie
4, place Jussieu
Paris

How to apply ?

Required Application Materials

1. Cover letter with current and future research interests
2. Most recent curriculum vitae
3. Copy of first author publications
4. Names and contact for three referees

How to submit

Interested candidates should

- Contact for additional information about the offer:
  Pr. Pierre Monmarché (pierre.monmarche@sorbonne-universite.fr),
  Pr. Ludovic Goudenege (ludovic.goudenege@math.cnrs.fr)
  Pr. Fabio Pietrucci (fabio.pietrucci@sorbonne-universite.fr)

- submit the required application materials to:
  Pascal Frey, Agnieszka Miskiewicz (iscd@sorbonne-universite.fr)
  with the tile “ISCD Fellowship Application”.

Selection Procedure

Selection process

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1. Eligibility check: candidate’s compliance with the requirements of the offer will be checked on the basis of the information provided by the applicant.
2. Evaluation of CV: applicant’s CV and research proposals will be evaluated and ranked according to their merit.
3. Interviews of candidates: **short listed** candidates will be invited for an interview conducted by the selection committee.
4. Final decision: the selected candidate will be proposed the position. A reserve list of candidates may be identified in case of withdrawal of the selected candidate.

Please note that priority in individual applicant selection will be given to first-time fellows.

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Job Offer

Job Summary

Title, Job Position	Postdoctoral position: Simulating the formation of the SEI in Li-ion batteries
Research Field	Applied mathematics
Employer	Sorbonne Université Institut des sciences du calcul et des données
Location :	Paris, France
Application Deadline / Timezone	15-02-2020 11:00AM Paris (GMT+01 :00)
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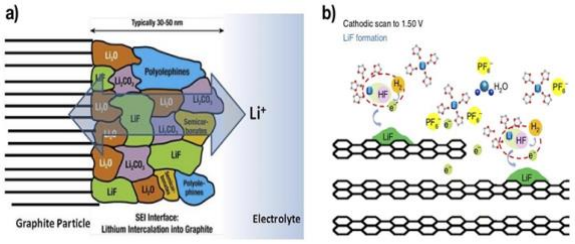
Offer description

Description

Scientific context. There are numerous situations for which one needs to study phase transitions and chemical reactions efficiently for characterizing energy materials. We will focus on a key aspect that governs the efficiency of batteries and their stability over time: The formation of the so-called solid electrolyte interphase (SEI). It is a complicated mixture of inorganic and organic components resulting from the reduction of the electrolyte during the first few cycles, as shown on Figure 1a). It is electronically insulating, but ionic conducting, thus allowing the passage of Li+ ions. Its stability is crucial for the operation of the Li-ion battery.



Controlling the SEI formation is one of the main objectives of current experimental research on batteries, and it will be one of the main topics of the Battery 2030+, a large-scale initiative which is currently being set up by European Union. The formation of the SEI consists in many steps, i.e. successive chemical reactions triggered by the strong electric fields at the interface and precipitation of several organic and inorganic salts within the electrolyte (which is made of a Li-PF6 salt dissolved in an organic carbonate solvent). Based on experimental evidence (Figure 1b), the precipitation of LiF at the surface of graphite electrodes is one of the first processes involved [Liu19]. **We will therefore perform simulations of the crystallization of this inorganic salt** in the carbonate solvent, both in the bulk and at graphite surfaces. We will adapt our method based on the use of permutation invariant vector-based path coordinates [Pipolo17, Fitzner17] to obtain first reactive trajectories. As a starting point, we will consider the classic (and computationally less expensive) problem of ion pair association and dissociation in solution, comparing the most recent advances in terms of collective variables and features of the projected dynamics [Ballard12, Mullen14, Salanne17] with the new results obtained within our project.

[Ballard12] A.J. Ballard, C. Dellago, Toward the Mechanism of Ionic Dissociation in Water, J. Phys. Chem. B 116, 13490 (2012).

[Fitzner17] M. Fitzner, G.C. Sosso, F. Pietrucci, S. Pipolo, A. Michaelides, Pre-critical fluctuations and what they disclose about heterogeneous crystal nucleation, Nat. Commun. 8, 2257 (2017)

[Liu19] T. Liu et al., In situ quantification of interphasial chemistry in Li-ion battery, Nature Nanotech 14, 50 (2019).

[Mullen14] R.G. Mullen, J.E. Shea, B. Peters, Transmission Coefficients, Committors, and Solvent Coordinates in Ion-Pair Dissociation, J. Chem. Theory Comput. 10, 659 (2014).

[Pipolo17] S. Pipolo, M. Salanne, G. Ferlat, S. Klotz, A.M. Saitta, F. Pietrucci, Navigating at will on the water phase diagram, Phys. Rev. Lett. 119, 245701 (2017).

[Salanne17] M. Salanne, S. Tazi, R. Vuilleumier, B. Rotenberg, Ca2+-Cl− Association in Water Revisited: the Role of Cation Hydration, Chem. Phys. Chem. 18, 2807 (2017).

Project PI: A. Marco SAITTA

Postdoc supervisors: A. Marco SAITTA – Mathieu SALANNE – Fabio PIETRUCCI

Appointment Term

Eighteen-months appointment starting as soon as possible.

Keywords: Nucleation, solvation, ionic compounds

As part of your duties, you may be required to provide internal training related to your business expertise.

Profile Requirements

Required Education Level

Expertise in molecular dynamics, statistical physics, free-energy methods, ab initio calculations

Skills / Qualifications

- Applicants must have a recent Ph.D. in Physics, Chemistry, or Materials Science
- Prior experience and proficiency in statistical physics, atomistic computer simulations, theoretical and computational modeling
- Applicants should be hard working, analytical and have excellent writing and communication skills necessary to author technical and scientific reports, publications, and deliver scientific presentations, seminars, meetings and/or teaching lectures
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  Pr. Marco Saitta (marco.saitta@sorbonne-universite.fr)
  Pr. Mathieu Salanne (mathieu.salanne@sorbonne-universite.fr)
  Pr. Fabio Pietrucci (fabio.pietrucci@sorbonne-universite.fr)

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