Laboratoire d'Electrochimie
et de Physico-chimie des Matériaux et des Interfaces
(UMR 5279)

LEPMI – Antenne Phelma Campus
1130 rue de La Piscine – BP 75
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https://lepmi.grenoble-inp.fr/

**Postdoctoral Position – Molecular Simulation for Solid-State Battery Electrolytes**

Location: Grenoble, France (LEPMI & CEA IRIG/MEM)
Duration: 18 months
Start Date: Autumn 2025 (flexible)

**Project overview :** Solid-state batteries represent a major technological step forward, combining improved safety and energy density. However, their development is hindered by complex interfacial phenomena and transport limitations within porous composite electrodes. Our project addresses these challenges by combining advanced experimental techniques with molecular modeling and data analysis, to provide a complete understanding of ion dynamics at the molecular scale.

**The appointed postdoc will lead the computational work**, developing molecular models of electrolytes based on polymers, LiFSI salt, and ionic liquids, in contact with active material surfaces. Simulations will be carried out in confined geometries representative of real electrodes, with the goal of understanding the impact of structure, composition, and interfaces on lithium transport.

**Profile of the ideal candidate**

We are looking for a junior researcher with the following qualifications:

- PhD in Physics, Chemistry, Materials Science, or a related discipline, awarded within the past two years.
- Solid experience with molecular dynamics (MD) simulations and classical force fields (e.g., LAMMPS, GROMACS).
- Familiarity with polymer and ionic systems, surface interactions, and ion transport is strongly desirable.
- Good command of scientific programming (e.g., Python, C/C++) and scripting for simulations and data analysis.
- Interest or experience in AI/ML tools applied to physical modeling (e.g., clustering, dimensionality reduction, surrogate models).
- Strong academic writing skills and clear communication abilities in English.

**Scientific environment in Grenoble**

The postdoc will work jointly between two leading research groups in Grenoble, and the work will be carried out in collaboration with an experimental post-doctoral fellow.

1. LEPMI (Laboratoire d'Électrochimie et de Physico-chimie des Matériaux et des Interfaces), a UMR research unit with recognized expertise in electrolyte elaboration, electrochemical characterizations, and operando measurement for energy storage.
2. MEM (Modeling and Exploration of Materials) group at CEA-IRIG, with internationally recognized contributions in molecular simulation of electrolytes and nanoconfined systems.

This position offers an exceptional multidisciplinary environment with close collaboration between simulation and experiment, access to high-performance computing resources, and interactions with researchers at LiPhy (B. Coasne) and across the Université Grenoble Alpes ecosystem.

**Contacts**
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