

## PhD position in atomic-scale modelling of ionic-liquids at interfaces

**Keywords:** Ionic liquids, confined fluid modelling, molecular mechanics, quantum mechanics, energy storage, material science, (ab-initio) molecular mechanics, Density Functional Theory, deep learning.

**Starting date:** September/october 2022 (3 years)

**Location:** [Institut des Matériaux de Nantes Jean Rouxel \(IMN\)](#) / [Nantes Université](#), France.

**Team / thematics:** [Physics of materials and nanostructures](#) / [Confined ionic liquids, ionogels](#)

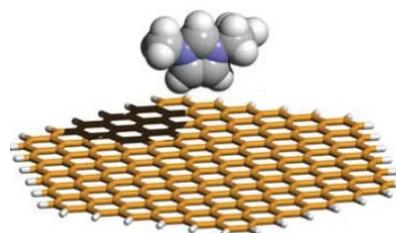
**Funding:** [École doctorale 3M](#)

**Advisor:** Jean Le Bideau

**Co-advisors:** Yann Claveau, Chris Ewels

### Context

This PhD will develop **QM/MM modelling of confined ionic liquids (ILs)**, led by [Yann Claveau](#) (new lecturer in the PMN group in 2021) and [Jean Le Bideau](#) (head of confined liquids research in the lab).



[RSC Adv., 2014, 4, 18017](#)

ILs exhibit very interesting properties useful for fields including **iontronics**, **catalysis**, **healthcare-related devices** and **energy storage (enhanced safety)**. Counter-intuitively, **confining ILs** within a host matrix (a process under development for “all-solid” batteries and other devices) can significantly increase their **ionic conductivity**. The mechanism driving these effects is not yet understood.

This PhD position will aim to understand the underlying physico-chemical mechanisms at host / IL interfaces using multi-model (Quantum Mechanics / Molecular Mechanics) multi-scale (from Å to μm, from ps to μs) simulations, in order to develop optimal ionic conductivity in ionogel electrolytes. The problem will be tackled through two complementary approaches: **modelling**, to understand, and **deep learning**, to produce data.

## Applicant Profile

- An excellent background in materials physics / physical chemistry / nanoscience (ranked in the top tier).
- Experience of atomic-scale modelling is a bonus: MD (LAMMPS) or DFT.
- Experience in programming is required.
- A strong sense of curiosity and exploration, preferring to try and fail sometimes rather than “sticking to the path”.
- Fluency in written and spoken English. French is an advantage but not essential.
- A team player with the ability and desire to collaborate with students on related projects.

Candidates should send a covering letter explaining why they are interested in the post, along with a comprehensive CV, to [yann.claveau@cnrs-imn.fr](mailto:yann.claveau@cnrs-imn.fr). “Standardised letters” not specific to this position will not be considered. There are no restrictions to applying based on nationality, and we are a committed equal opportunities employer. Closing date for application: 11th July 2022.

