MASTER INTERNSHIP

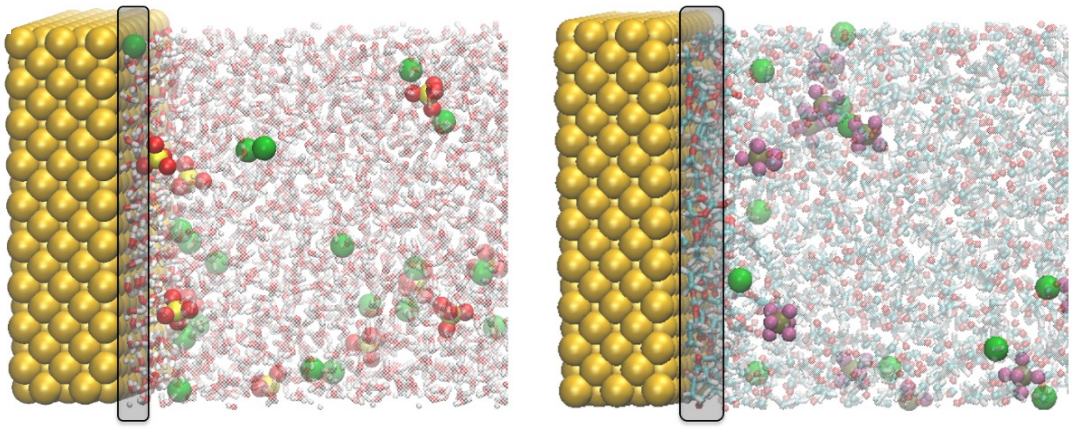
PHENIX

SORBONNE UNIVERSITÉ

cnrs

Simulation of high potential electrolytes for Li-ion batteries

The Li-ion battery is now a mature technology. However, its large-scale deployment poses availability problems for critical elements, in particular cobalt, which is used in cathode materials. One possibility is to use compounds based on manganese oxide. Since these materials display higher intercalation potentials, they would also increase the amount of stored energy, but it is then necessary to use stable electrolytes over wide ranges of potentials. Among the avenues explored the use of fluorinated salts with bis(fluorosulfonyl)imide (FSI) as anion [1] is promising, but these tend to corrode aluminum current collectors.



In order to better control these corrosion phenomena, it is necessary to understand them at the molecular level. During this internship, we will study the structural properties (ion solvation, short- and long-range structure) of a liquid composed of the LiFSI salt dissolved in carbonate type solvents on the surface of a metallic aluminum current collector. For this, we will use classical molecular dynamics, which is a numerical simulation method where molecules and materials are described at the atomic scale.

Our team has recently developed simulation software [2] that allows us to study electrode/electrolyte interfaces with precision. It has been used in particular to study energy storage devices such as supercapactitors [3] metal-ion batteries [4]. The work will be performed on national and european high-performance computers.

[1] B. Aktekin et al., Concentrated LiFSI-Ethylene Carbonate Electrolytes and Their Compatibility with High-Capacity and High-Voltage Electrodes, ACS Appl. Energy Mater., 2022, 5, 585.

[2] A. Marin-Laflèche et al., MetalWalls: A classical molecular dynamics software dedicated to the simulation of electrochemical systems, J. Open Source Softw., 2020, 5, 2373.

[3] M. Salanne et al., Efficient storage mechanisms for building better supercapacitors, Nature Energy, 2016, 1, 16070.

[4] P. Lemaire et al., Probing the Electrode–Electrolyte Interface of a Model K-Ion Battery Electrode─ The Origin of Rate Capability Discrepancy between Aqueous and Non-Aqueous Electrolytes, ACS Appl. Mater. Interfaces, 2022, 14, 20835.

Period: February 2023 - July 2023 (dates can be adapted)

Specific techniques or methods: Molecular dynamics simulations

Candidate Profile: Strong background in physical chemistry or material science

Follow-up PhD thesis: Yes (through a collaboration with an industrial partner)

Application: Please send a CV and a motivation letter to Mathieu Salanne

Contact: mathieu.salanne@sorbonne-universite.fr

Sorbonne University is a world-class, research-intensive university bringing together a broad range of arts, humanities, social sciences, natural sciences, engineering and medicine. The scientific Pierre and Marie Curie campus was completely refurbished in 2016.

PHENIX is a laboratory at the interface between Chemistry, Physics and Materials Science with a long-standing expertise of colloidal systems, electrolytes and fluids under confinement. Its strength lies in a combination of experimental and modelling activities (numerical simulations). Several international projects and networks are in place in PHENIX, providing a rich and multinational environment.