AMÉLY RONDEAU

PhD student in computational chemistry

PhD researcher in molecular modeling of solid-state electrolytes for Li-ion batteries. Strong background in materials chemistry with specialization in molecular dynamics, forcefield optimization, and machine learning. Skilled in computational chemistry with a multidisciplinary, research-oriented mindset

Nanterre, France

+33 (0)6 95 10 77 66
amely.rondeau@gmail.com

ADDITIONAL SKILLS

Language

- French: native speaker
- English: advanced
- German: basic knowledge

Programming

Python, R, Matlab, Perl

Computational chemistry

- Molecular dynamics, forcefield optimization, DFT
- Property predictions (diffusivity, ionic conductivity, cohesive ernergy, density)

Software and Tools

- Materials Studio, Ovito, Gulp LAMMPS, GROMACS
- Pipeline Pilot

ADDITIONAL EXPERIENCES

In charge of publication for the Forum Horizon Chimie 2022

- Designed the brochure
- Sollicited companies
- Conducted alumni interview

Vice-president of the PhD student association (ADIFP): organize social events, contact companies

EXPERIENCES

IFP Energies nouvelles, Rueil-Malmaison, France — **Nov 2024 -**
PhD student

Studied and optimized classical and machine learning forcefield to accurately describe lithium ion diffusion in solid-state electrolytes (halide and hybrid materials). Employed molecular dynamics methods to calculate ionic conductivity and diffusivity. Analyzed simulated structures using radial distribution function, XRD, phonons, mechanical properties and entropy-based tools.

- Oral presentation at the 42nd Topical Meeting of ISE (june 2026): "*Comparative analysis of Classical and Machine-Learning Potentials for Ionic Transport in Halide Solid-State Electrolytes*"

Dassault Systèmes, Vélizy-Villacoublay, France — **February - July 2024**
6-month internship

Studied and optimized classical forcefield utilized for modelling crystal structures in Materials Studio sofware. Employed molecular dynamics methods to calculate properties of structures previously cleaned from the Cambridge Structural Database. Evaluated outcomes by comparing them with DFT values and experimental data. Regular meetings with the R&D team in Cambridge

Karlsruher Institut für Technologie (KIT), Karlsruhe, Germany — **April - August 2023**
4-month internship

Developed machine learning models trained on experimental data about the UV response properties of hydrogels Developed generic monomer representations for improved generalisation to predict properties of hypothetical hydrogels based on unseen monomers

Prysmian Group — **Sept. 2022 - March 2023**
Project leader of a 9-people group

Coordinated a project between Prysmian Group and the European School of Chemistry Polymers and Materials. Analyzed state-of-the-art manufacturing technologies and proposed adaptations for the optical cable sector.

EDUCATION

PhD — **2024-2027**
Sorbonne Université, Paris, France

Molecular modeling of polymer-electrolyte interfaces in hybrid-solid battery applications

Master's Degree in Material Engineering and Nanoscience — **2023-2024**
University of Strasbourg, France

Studied materials for health and environment
Materials for data storage, solar energy harvesting and electrochemical storage and conversion

Master's Degree in Engineering MSc — **2021-2024**
ECPM (European school of chemistry, polymers and materials), Strasbourg, France

Artificial Intelligence and Chemistry specialization - Material chemistry specialization
Programmed algorithms to identify molecules in UV-vis spectra during a group project. Assimilated material properties and their use. Conducted several pratical works.