Master thesis proposal

Modeling halide electrolytes for solid-state batteries with machine learning interatomic potentials

Keywords : Solid-state batteries, Machine learning interatomic potentials, atomistic simulations

SCIENTIFIC DESCRIPTION :

Solid-state batteries (SSBs) represent a promising solution for next-generation energy storage, offering higher energy density and improved safety compared to conventional liquid electrolyte Li-ion cells. To advance the development of SSBs, this internship project will employ machine learning approaches and in-house developed workflows to accurately and efficiently predict the properties of solid-state electrolyte materials.

The internship will focus on ternary metal halides, a family of solid electrolytes known for their high ionic conductivity [1]. The trainee will investigate lattice dynamics through phonon dispersion calculations and explore ionic transport mechanisms using molecular dynamics (MD) simulations to determine Li-ion diffusion coefficients and energy barriers. The goal is to provide deep insights into the ion diffusion mechanisms that govern ion transport and to assess their structural stability under various temperature and pressure conditions.

For this purpose, the trainee will utilise our configurable workflow, which automates dataset generation from density functional theory (DFT) calculations, to fine-tune several universal machine learning interatomic potentials (MLIPs), including CHGNet [2], Sevennet [3], and PET-MAD [4]. The impact of fine-tuning on the accuracy and transferability of these MLIPs will then be quantified. Benchmark and validation will be essential components of the project, involving comparison between DFT results and predictions from fine-tuned MLIPs across various materials properties, including lattice constants, phonon dispersions, and Li-ion diffusion coefficients.

We are seeking a Master 2 student in Materials Science, Chemistry, Physics, or a related field, with a solid background in solid-state chemistry and materials science. The ideal candidate should have hands-on experience with UNIX (bash/shell scripting) and Python. Familiarity with atomistic simulation packages such as VASP, Quantum ESPRESSO, and LAMMPS is a plus. Most importantly, we value curiosity and strong communication skills.

References:

[1] Zheng, Anyi, et al. "Composition regulation of ternary rare-earth halide solid-state electrolytes and its influence on their ionic conducting and electrochemical properties." *Journal of Materials Chemistry A* 13.8 (2025): 6067-6074.

[2] Deng, Bowen, et al. "CHGNet as a pretrained universal neural network potential for charge-informed atomistic modelling." *Nature Machine Intelligence* 5.9 (2023): 1031-1041.

[3] Kim, Jaesun, et al. "Data-efficient multifidelity training for high-fidelity machine learning interatomic potentials." *Journal of the American Chemical Society* 147.1 (2024): 1042-1054.

[4] Mazitov, Arslan, et al. "PET-MAD, a universal interatomic potential for advanced materials modeling." *arXiv preprint arXiv:2503.14118* (2025).

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Techniques/methods in use : DFT simulations, high-performance computing (HPC), use and fine-tuning of universal MLIPs, large-scale MD simulations, Python-based data analysis, management of large datasets, and scientific communication.

Budget description and use : Internship compensation (CNRS) and acquiring a computer

Applicant skills : Python coding, Interest in computational materials science and solid-state batteries, willingness to work with computational tools on linux (bash/shell scripting) and large dataset, Simulation packages (such as VASP, Quantum ESPRESSO, and LAMMPS).

Internship supervisors : Bassem SBOUI, bassem.sboui@icmcb.cnrs.fr, +33 5 40 00 66 27
Aurélie CHAMPAGNE, aurelie.champagne@icmcb.cnrs.fr, +33 5 40 00 26 47

Internship location : Institut de Chimie de la Matière Condensée de Bordeaux (ICMCB) UMR5026, Group 2 at ENSMAC, "GEMBATT ", 16 Av. Pey Berland 33607 Pessac

Possibility for a Doctoral thesis : ~~Yes~~/No