

Master thesis proposal

Atomistic investigation of liquid metals in the context of nuclear accident scenarios

Keywords : Liquid metals, atomistic simulations, machine-learning interatomic potentials

SCIENTIFIC DESCRIPTION :

In the context of nuclear accident scenarios, liquid mixtures may form, containing uranium, zirconium, and elements from structural materials and the reactor vessel (such as steel). Understanding the relationship between the properties of these mixtures—particularly their viscosity—and their structural characteristics is therefore crucial.

Atomistic investigations have already been conducted on liquid uranium-zirconium mixtures, successfully establishing predictive models for these relationships. The approach used relies on developing machine-learning interatomic potentials based on *ab initio* calculations, which are then employed to perform large-scale classical molecular dynamics simulations.

However, the lack of experimental data for these specific compositions makes it challenging to validate the proposed methodology. During this internship, the candidate will focus on simulating compositions that remain relevant to nuclear accident scenarios—such as zirconium-nickel or zirconium-iron—but have been more thoroughly studied experimentally. The goal is to directly compare model predictions (e.g., thermal expansion, liquid structure, and atomic diffusion) with available experimental measurements.

This work will contribute to validating the methodologies used for simulating liquid mixtures, thereby enhancing their reliability for nuclear safety applications.

Techniques/methods in use : atomistic simulations, density functional theory (DFT) and classical molecular dynamics calculations, development of machine-learning interatomic potentials, structural analysis of liquid systems.

Budget description and use : Salary for the student

Applicant skills : We are seeking for motivated applicants with a background in materials simulations and statistical physics.

Industrial partnership : None

Internship supervisor(s) : Julien TRANCHIDA, julien.tranchida@cea.fr, 0611345881, Work-Package leader in the Fast-In-Fuel Project

Internship location : CEA Cadarache

Possibility for a Doctoral thesis : Yes

