

# Exploring Thermal Disorders and Ultraconfined Water Dynamics in C-S-H at High Temperatures

Supervisors:

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## Project Description

This 6-month internship focuses on modeling the thermally-induced changes in the molecular structure of Calcium-Silicate-Hydrate (C-S-H), along with a comprehensive analysis of the dehydration reactions at high temperatures. This internship is a precursor to an upcoming Ph.D. thesis project that will be starting in the fall of 2024.

The selected candidate will play a key role in the initial exploration phase of our thesis project, specifically studying the effects of high temperatures on the molecular structure of C-S-H. This involves using advanced molecular simulations to investigate the impact of high temperatures on the molecular structure of C-S-H, with a specific focus on understanding thermal-induced responses and chemical composition variations. Special attention will be directed towards understanding the behavior of ultra-confined water within the C-S-H gel under elevated temperature conditions, contributing valuable insights to the overall research initiative.

## Internship Highlights

- 1. Molecular Dynamics Skillset:** Conduct advanced molecular simulations to model and analyze the behavior of C-S-H at the molecular level. Develop skills in the molecular calculation code '[LAMMPS](#)', use MATLAB for pre- and post-processing, and gain familiarity with visualization tools such as VMD and Avogadro
- 2. Collaborative Environment:** Work closely with our experienced research team at the 3SR laboratory, benefiting from an innovative research environment that integrates experimental studies, encompassing X-ray and neutron tomography (See [Next](#)), with multi-scale modeling spanning from the nanoscale to the macroscale.

**3. Link to ANR Project:** Contribute to the goals of the ANR project "MULTI-FIRE," gaining insights into the larger context of multiscale modeling in materials science.

**4. Prospects for extending into Ph.D. thesis:** The successful intern is encouraged to extend his involvement and continue working beyond the internship period on the broader thesis project starting in the fall of 2024.

## Requirements

- Master's students in their second year or final-year engineering students.
- Background in Physics, chemistry, Materials Science, or a related field.
- Strong motivation for conducting molecular simulations.
- Familiarity with molecular dynamics is appreciated but not mandatory.

## Internship Duration and Location

6 months internship starting from February 2024 at [the 3SR lab](#) in Grenoble.

## Application process

Please submit your application including motivation letter and CV to M. Laanaiya - [majdouline.laanaiya@univ-grenoble-alpes.fr](mailto:majdouline.laanaiya@univ-grenoble-alpes.fr) or/and S. Dal Pont - [stefano.dalpont@3sr-grenoble.fr](mailto:stefano.dalpont@3sr-grenoble.fr) before January 15st, 2024.