Molecular Dynamics of C-SH

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Objectives:
The purpose of this research is to study adsorption of ions such as magnesium, aluminum, and sulfate onto the surface and into the structure of C-S-H by combining molecular dynamic and metadynamics simulations.

Why molecular dynamics?

C-S-H is the glue of cement. Simulation of C-S-H by means of molecular dynamic simulation will help to understand mechanism of adsorption of ions and consequently change in morphology of C-S-H since experiments have shown ions such as sulfate dramatically change the morphology of C-S-H

Simulations and force fields

In order to perform each molecular dynamics simulation we need a force field to be used. A force field is a set of inter-atomic potentials that describes the behavior of a system. We are using LAMMPS code and three ERICA force fields to perform our simulations.

ERICA Force Fields

We developed three force fields, ERICA FF1 is a combination of three force fields, ERICA FF2 is a combination of six, and FF3 is a combination of eight different force fields. Additionally force fields were validated by the simulation of many cementitious systems, reaction enthalpies, and the simulations of ions in water.

How does ERICA FF2 simulate toborite?

Tobomorite is a natural mineral which is very similar to C-S-H. Experimental findngs show that Ca in the main layer of tobomorite has a 7-fold coordination by oxygen of silicon and oxygen of hydroxyl. ERICA FF2, a force field validated by the simulation of 14 cementitious systems and 17 reaction enthalpies, correctly simulates the 7-fold coordination of tobomorite.