I. Introduction

- **Application 1:** The Al-rich species constitute up to 15 wt.% of cement paste. **Issue:** Early Ettringite Formation (EEF) and Delayed Ettringite Formation (DEF) that cause undesirable cracking and deterioration of cement-based materials.
- **Application 2:** The Al-rich species are used as a binder for hazardous waste encapsulation. **Issue:** Strength requirement for efficient stabilization of heavy ions.

II. Motivations and Objectives

- Interpret the findings at large length scales based on the structural response and failure mechanisms that occur at the nano-scale.
- Understand the mechanical properties of the Al-rich species that are detrimental to control the strength development in a range of common cementitious materials.

III. Methodology: Atomistic Simulation

- **Initialization:** Setup atomistic model; define initial atomic positions and velocities; define reactive force field (ReaxFF); energy minimization
- **Reactive Molecular Dynamics:** Calculate forces; update atomic positions and velocities, iterate until thermodynamic equilibrium is reached
- **Uniaxial Tension Straining:** Strain simulation cell in a Cartesian direction; remap positions of atoms; relax lateral directions, repeat until permeant failure occurs
- **Post-Processing:** Collect trajectories, determine stress-strain relationships

IV. Atomistic Models of Al-Rich Species of Hydrated Cement

- Hydrogarnet
- Ettringite
- Monosulfoaluminate

V. Hydrogarnet: Failure Mechanism

- In x, y, and z directions:

VI. Ettringite: Failure Mechanisms

- In x and y directions:
- In z direction:

VII. Monosulfoaluminate: Failure Mechanisms

- In x and y directions:
- In z direction:

VIII. Conclusions and Future Works

- The presented results are expected to directly contribute to understand how the strength and stiffness of the Al-rich species of hydrated cement can be improved based on the fundamental mechanical behavior captured at the atomic scale.