

## Defense Announcement

*Molecular Crosslinking of Calcium-Silicate-Hydrate with Organosilanes: Toward Engineering of Cementitious Matrices with High Thermal Resistance*

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**Degree:** Ph.D. Civil Engineering

**Date:** 05/19/2021

**Time:** 1:00 PM - 3:00PM

**Location:** Zoom

**Meeting ID:** 970 9338 8462

**PIN:** 327000

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This research work is focused on the development of a novel approach aiming at improving the thermal resistance of cementitious matrices. The proposed approach utilizes the molecular scale crosslinking phenomena in which the galleries of inorganic calcium-silicate-hydrate (C-S-H), the main product of cement hydration, are directly bridged with bis-organosilanes molecules. The crosslinking with organic molecules provides C-S-H with attributes imperative for the reduced thermal conductivity e.g. contrast in vibrational densities of states and reduced particle density, which can positively alter the insulation potential of cement-based matrices at a macro-scale. It is postulated, that such a solution can be successfully realized at an engineering scale in the form of a high concentration seed admixture applied to hydrating cement mixtures. The results reported in this research demonstrate the feasibility of the proposed crosslinking approach; the organic-inorganic C-S-H gels of controlled stoichiometry can be successfully realized via sol-gel processing and using bis-alkoxysilanes of various lengths of the alkyl chain.

The results of the extensive experimental campaign show that the novel organic-inorganic gels have layered turbostratic molecular structure with certain similarities to C-S-H precipitating in hydrating cement paste. The organic molecules' chain length controls the interlayer distance, which shows little to no shrinkage upon dehydration up to 105 °C. However, the structure of hybrid C-S-H becomes distorted in the basal plane, in which dimer and trimer Si-polyhedra structures condense on a 2D hexagonal Ca-polyhedra layer. Cross-linked C-S-H gels display plate-like morphology with a tendency toward stacking into agglomerates at a larger scale. Hybrid organic-inorganic C-S-H gels exhibit significantly lower intrinsic conductivity than the inorganic one and the magnitude of the observed reduction is related to the molecular size of the bis-organosilanes. The largest reduction was achieved for the organic-inorganic C-S-H incorporating the longest chain organic molecules ( $nCH_2=8$ ).

The results of isothermal calorimetry confirmed the positive action of inorganic and hybrid C-S-H seeds on the hydration of type II cement system. Both types of seed incorporation to the cement system lead to the increased intensity on the onset of the hydration reaction as well as

higher heat rates of main hydration peaks. Also, higher total heat of hydration resulted from the incorporation of the C-S-H seeds, thus indicating enhanced formation of hydration products; hybrid C-S-H seeds displayed superior activity in comparison to the inorganic seed. XRD test results revealed that the addition of both types of seeds did not alter the types of hydration products formed in the hardened paste; especially in the case of hybrid seeded cement system, it was observed that seeds have been efficiently accommodated in the system as a whole and tend to be chemically stable, which also supported by thermal analysis.