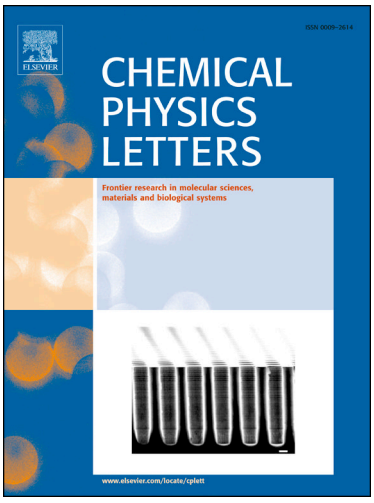


Research paper

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# Reactive Molecular Simulation on the Calcium Silicate Hydrates/Polyethylene Glycol composites

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## Abstract

Calcium silicate hydrates (C-S-H) may potentially exhibit extraordinary performance when modified by polymers, in which way the properties of cement-based materials can be improved from the genetic level. In this molecular dynamics simulation of the interaction between C-S-H and polyethylene glycol, apart from the H bond network connection in the interface, another chemical adsorption was observed. Calcium of C-S-H broke the C-O bond of PEG and formed a new Ca-C connection, which created a stronger link between the organic and inorganic phases.

Key words: calcium silicate hydrates; polyethylene glycol; molecular dynamics; adsorption