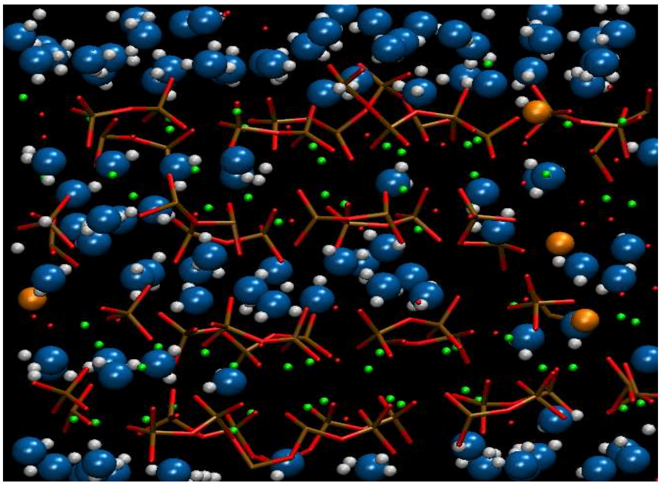
Locking Mercury into Concrete

Problem

There is an ongoing debate between industry and federal regulators whether coal fly-ashes should be regulated as hazardous materials. Due to the mixture of calcium and aluminum it contains, fly ash is an excellent candidate to partially replace portland cement, and thus a viable economical and ecological solution. Research at MIT has identified that the substitution of aluminum for calcium in the fundamental building block of concrete, the calcium-silicate-hydrates (C-S-H), enhances strength and durability. Fly ash, however, is known to contain naturally occurring trace concentrations of mercury and other heavy metals, which raises important environmental concerns. From a concrete science perspective, it is thus important to pin down the way mercury is locked into C-S-H, when cement blended with fly ash reacts with water to form cement hydrates. The key question to be addressed is how the incorporation of mercury in C-S-H affects its long-term structural and chemo-mechanical stability. Answering this question is critical to balance effective use of materials with environmental concerns, with high economical and ecological pay-offs for industry and society at large.



Molecular model of mercury (Hg^{2+}, orange spheres) incorporation in Calcium (green) – Silicate (red-brown sticks) – Hydrates (blue-white spheres).

Approach

In contrast to classical empirical approaches that hint towards the chemical stability of heavy metals bound in cement hydrates, we have chosen a bottom-up approach that starts at the electron and atomic scale of cement hydrates with calcium-mercury (Ca-Hg) substitutions. Based on first principles of ion coordination, mercury in the ionic Hg^{2+} electronic state is recognized to substitute for calcium atoms in the C-S-H molecular structure. Energy minimization of a large range of molecular structures with varying mercury concentration confirms the stability of this solid mercury adsorption, and provides a means to probe the mechanical properties of molecular structures at fundamental scales.

Findings

The key finding of this research is that a stable C-S-H structure is maintained for a Ca-Hg substitution of up to 10% (in number of atoms) compared to normal C-S-H. In particular, below 2% of substitution, the mechanical properties are unaffected by the mercury adsorption. Above 2%, there is a degradation in elastic properties of the Hg-containing compounds, which reaches 30% for the highest, still stable configuration.

Impact

This research suggests that C-S-H can safely host mercury (Hg^{2+}) while maintaining full chemical stability and mechanical performance, when less than 2% of calcium sites are exchanged for mercury. To fully recap the benefits of higher strength and durability of concrete with high fly ash concentrations, it may turn out beneficial to limit the mercury content in fly ashes for concrete.

More

Research presented by Drs. R.Pellenq and F-J.Ulm.

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