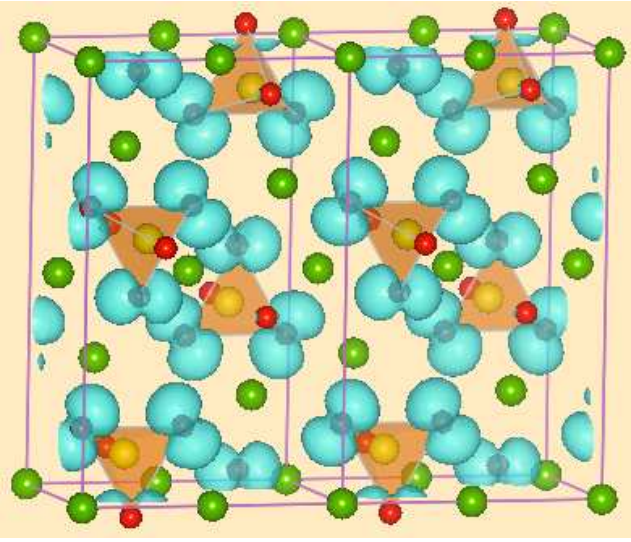
Concrete Sustainability Hub@MIT Research Profile Letter – October 2010

Quantum Clinker Engineering

Problem

One potential game changer identified by the cement industry to reduce the environmental footprint, is the implementing of strategies for the activation of lower greenhouse components such as belite. Indeed, such a shift from alite to belite dominated portland cement systems has two advantages: it entails a lowering of the processing temperature in clinker production, and reduces the amount of carbon-dioxide emitted in the de-carbonation of limestone. However, the key for an increase of belite concentration in industrial portland cement compositions is the increase of belite reactivity, including dissolution and precipitation rates. This requires the identification of the limiting stages of clinkers' dissolution chemistry. Clinker phases are crystals, in which chemical reactions occur at reactive sites on crystal planes that have the highest surface energy. In return, if surface energies on all crystal planes were known, dissolution rates could be engineered for specific clinker phases, impurities, crystal structure, and so on.



Electron clouds (light blue) in a belite crystal as obtained by Quantum Simulations. The green, yellow, and red spheres represent Ca, Si, and O atoms, respectively. The simulation box has dimensions of 5.1*11.3*6.8 Angstrom.

Approach

In contrast to classical bulk thermodynamic equilibrium concepts, that cannot recapitulate surface energy states, we have chosen a quantum mechanics approach that starts at electron scales to fully characterize the electronic structure, stability and reactivity of alite and belite, including the effects of impurities (e.g. magnesium). Conducting a wide range of quantum simulations in all possible directions of crystals of varying thickness, the first ever quantum cement surface energy characterization is achieved. These surface energies provide the critical link between crystallography and dissolution energetics of clinker phases.

Findings

The key finding of this research is that alite has one least stable/most reactive crystallographic plane (010). In contrast, belite has several planes of similar surface energies (111, 101, 001). On these surfaces, the energy required to detach (dissolve) calcium is roughly twice as much as in alite. This means that while alite has one preferential plane of dissolution, belite has several that are more stable and thus less reactive.

Impact

This research highlights the critical role of the crystal structure of alite and belite on the dissolution energetics. This novel understanding of the dissolution chemistry eventually holds the key to designing potential dissolution accelerators and retarders for the activation of lower greenhouse components such as belite so that they can be used in demanding construction schedules.

More

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