Hard facts lead to 'green' concrete

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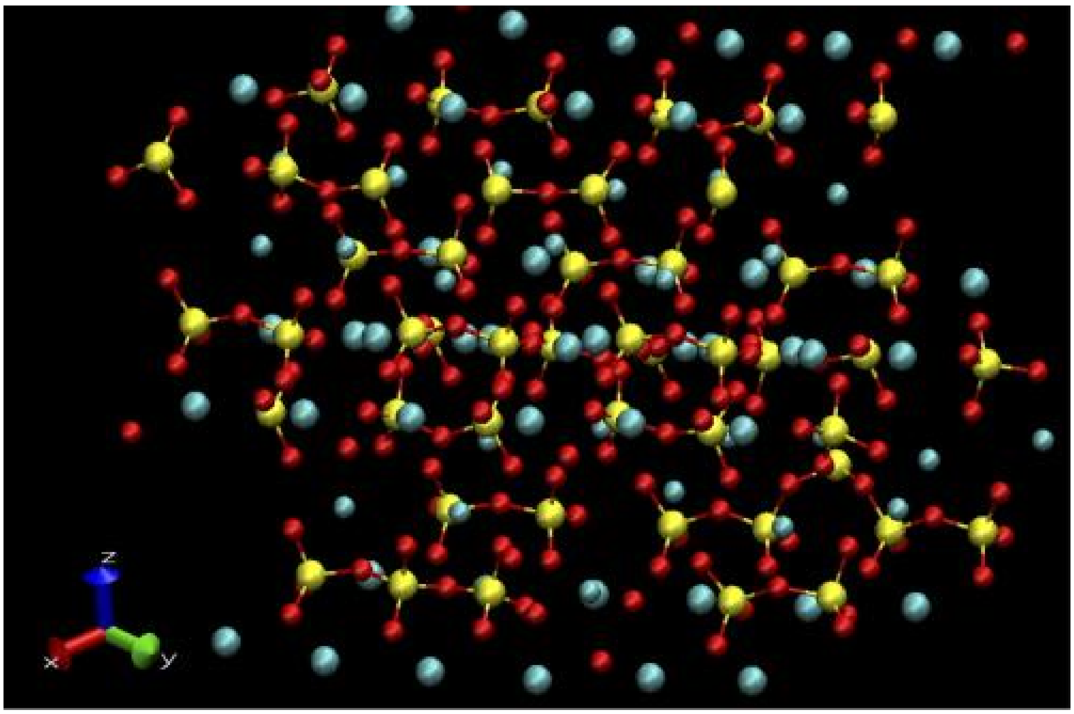

The generic molecular structure of cement consists of silicon (yellow) calcium (blue) and oxygen (red) atoms, with the addition of water molecules (not shown). A team of scientists including Rouzbeh Shahsavari of Rice University has created computational models to help concrete manufactures fine-tune mixes for specific applications Credit: Shahsavari Lab/Rice University

The international team of scientists has created computational models to help concrete manufacturers fine-tune mixes for general applications.

Rice materials scientist Rouzbeh Shahsavari said the team created what it considers a game-changing strategy for an industry that often operates under the radar but is still the third-largest source of carbon dioxide released to the atmosphere.

Nature Communications published the open-access study online this week.

The annual worldwide production of more than 20 billion tons of concrete contributes 5 to 10 percent of carbon dioxide, according to the researchers; only transportation and energy surpass it as producers of the greenhouse gas.

There are benefits to be gained for the environment and for construction by optimizing the process, said Shahsavari, an assistant professor of civil and environmental engineering at Rice. "The heart of concrete is C-S-H – that's calcium, silicate and hydrate (water). There are impurities, but C-S-H is the key binder that holds everything together, so that's what we focused on.

"In a nutshell, we tried to decode the phases of C-S-H across different chemistries, thereby improving the mechanical properties of concrete in a material way."

The yearslong study involved analysis of "defect attributes" for concrete, Shahsavari said. One was in the ratio of calcium to silicon, the basic elements of concrete. Another looked at the topology of atomic-level structures, particularly the location of defects and the bonds between "medium-range" calcium and oxygen or silicon and oxygen atoms – that is, atoms that aren't directly connected but still influence each other. The combination of these defects gives concrete its properties, he said.

Shahsavari noted a previous work by the team defined average chemistries of cement hydrates. (Cement is the component in concrete that contains calcium and silicon.)

"C-S-H is one of the most complex structured gels in nature, and the topology changes with different chemistries, from highly ordered layers to something like glass, which is highly disordered. This time, we came up with a comprehensive framework to decode it, a kind of genome for cement," he said.

The team looked at defects in about 150 mixtures of C-S-H to see how the molecules lined up and how their regimentation or randomness affected the product's strength and ductility.

The ratio of calcium to silicon is critical, Shahsavari said. "For strength, a lower calcium content is ideal," he said. "You get the same strength with less material, and because calcium is associated with the energy-intensive components of concrete, you use less rebar and you save energy in transporting the raw material. Also, it's more environmentally friendly because you put less carbon dioxide into the atmosphere."

Alternately, a higher ratio of calcium (indeed there is a sweet spot) provides more fracture toughness, which may be better for buildings and bridges that need to give a little due to wind and other natural forces like earthquakes or well cement subjected to downhole pressure or temperature variation.

"This is the first time we've been able to see new degrees of freedom in the formation of concrete based on the molecular topology," Shahsavari said. "We learned that at any given calcium/silicon ratio, there may be 10 to 20 different molecular shapes, and each has a distinct mechanical property.

"This will open up enormous opportunities for researchers to optimize concrete from the molecular level up for certain applications," he said.

"There has been a lot of work in metals and semiconductors, but understanding how defects work in cement was far from obvious, and there was pretty much no basic work done at this level.

"So I would say this is perhaps one of the most important discoveries in cement science this century."

More information: "Combinatorial molecular optimization of cement hydrates" *Nature Communications* 5, Article number: 4960 DOI: 10.1038/ncomms5960

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