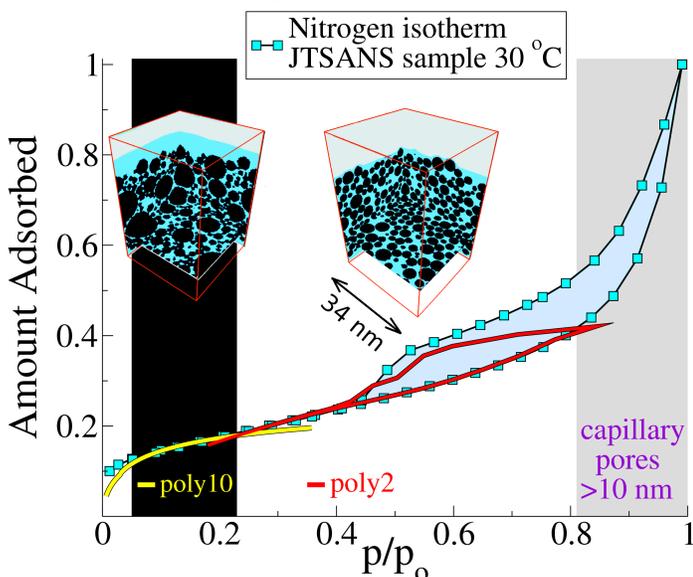


# C-S-H Texture From Sorption Isotherms

## Problem

The microstructure of cement paste forms by precipitation of products, the most important and abundant of which is C-S-H. Recent approaches to characterizing this microstructure have included models with disordered mesoporous networks that have various pore size distributions, and the comparison of these models to experimental gas sorption isotherms. Although, the hysteresis in cement paste adsorption/desorption isotherms were first observed decades ago, no models have been able to quantitatively predict those isotherms and be consistent with mechanical properties. This new bottom-up approach incorporates the mesoscale and permits verification of the model through direct comparisons with experimental data.



Comparison of experimental nitrogen sorption isotherm [exp. data from Dr. J. Thomas, Schlumberger Doll Research] with the theoretical results obtained using model C-S-H microstructures. “Poly2” and “Poly10” refer to low and high density C-S-H model microstructures, respectively.

## Approach

We perform a theoretical study of adsorption/desorption hysteresis by combining the mean-field density functional theory (DFT) with a coarse-grained lattice-gas model of C-S-H

microstructures<sup>1,2</sup>. To achieve this goal, a model of C-S-H microstructure is combined with a model of gas/liquid adsorption in a porous structure, which is capable of predicting sorption isotherms. We explore heterogeneous microstructures in terms of local densities and packing fractions that were generated via Grand Canonical Monte Carlo simulations of aggregation of nano-sized C-S-H grains with diameters ranging between 1 and 10 nm.

## Findings

We show that the combination of DFT with a simple lattice-gas model of the polydisperse C-S-H grains can reproduce major features of the experimental sorption isotherms. We identify three distinct regions in the adsorption/desorption curve: sorption at relative pressures below 0.25 P/P<sub>o</sub> is characterized by the highly polydisperse C-S-H grains with high density (packing fraction 75%) and narrow pores; sorption between 0.25 and 0.80 P/P<sub>o</sub> occurs in the less dispersed granular material with low density (packing fraction 66%) and wide range of pore size distribution; and above 0.80 P/P<sub>o</sub> the major contribution is due to the capillary pores whose distribution can be determined from the classic Kelvin equation.



## Impact

This unique bottom-up approach developed by the CSHub combines information from atomistic and colloidal simulations with the coarse-grained lattice-gas model allowing validation of the cement model structure at a larger length scale. This facilitates the first composite model of C-S-H at mesoscale, guiding the development of cement microstructures with desired mechanical properties.

## More

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1 E. Masoero *et al.*, Research Profile Letter - June 2011.

2 E. Masoero *et al.*, Research Profile Letter - November 2011.



This research was carried out by the CSHub@MIT with sponsorship provided by the Portland Cement Association (PCA) and the Ready Mixed Concrete (RMC) Research & Education Foundation. The CSHub@MIT is solely responsible for content. For more information, write to CSHub@mit.edu.