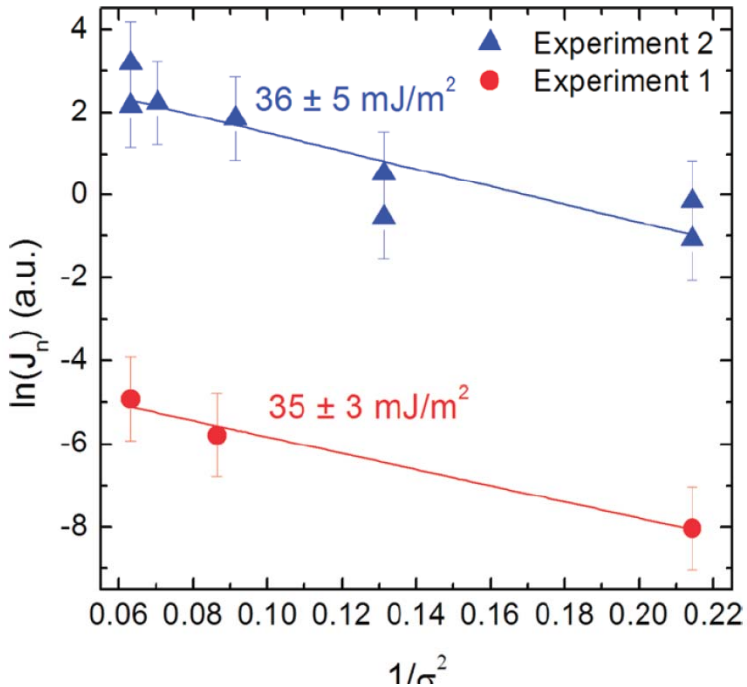
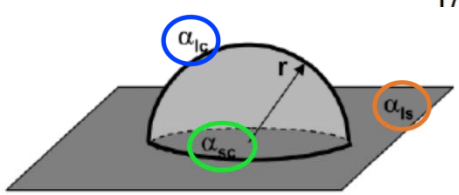
Determination of Interfacial Energies between $CaCO_3$ and Quartz





$$J_n = A\exp\left(-\frac{16\pi v_m^2 \alpha'^3}{3k_B^3 T^3 \sigma^2}\right)$$

$$\alpha' = \alpha_{lc}\{1-(\alpha_{ls}-\alpha_{sc})/2\alpha_{lc}\}$$

from DeYoreo and Vekilov (2003)

Interfacial energies of the water-$CaCO_3$-quartz system measured using a grazing incidence X-ray Small-Angle Scattering technique (APS beamline 12ID-B)

Measured value lower than that for homogeneous carbonate nucleation (36 vs 120 mJ/m^2) => $CaCO_3$ precipitation favored on quartz grain surfaces

Important information to help predict **where** $CaCO_3$ will precipitate in rocks and at what supersaturation; this in turn will allow prediction of changes in permeability, not just changes in porosity

Fernandez-Martinez, A., Hu Y., Lee B., Jun Y.-S. and Waychunas G.A. Environ. Sci. & Tech., DOI:10.1021/es3014826

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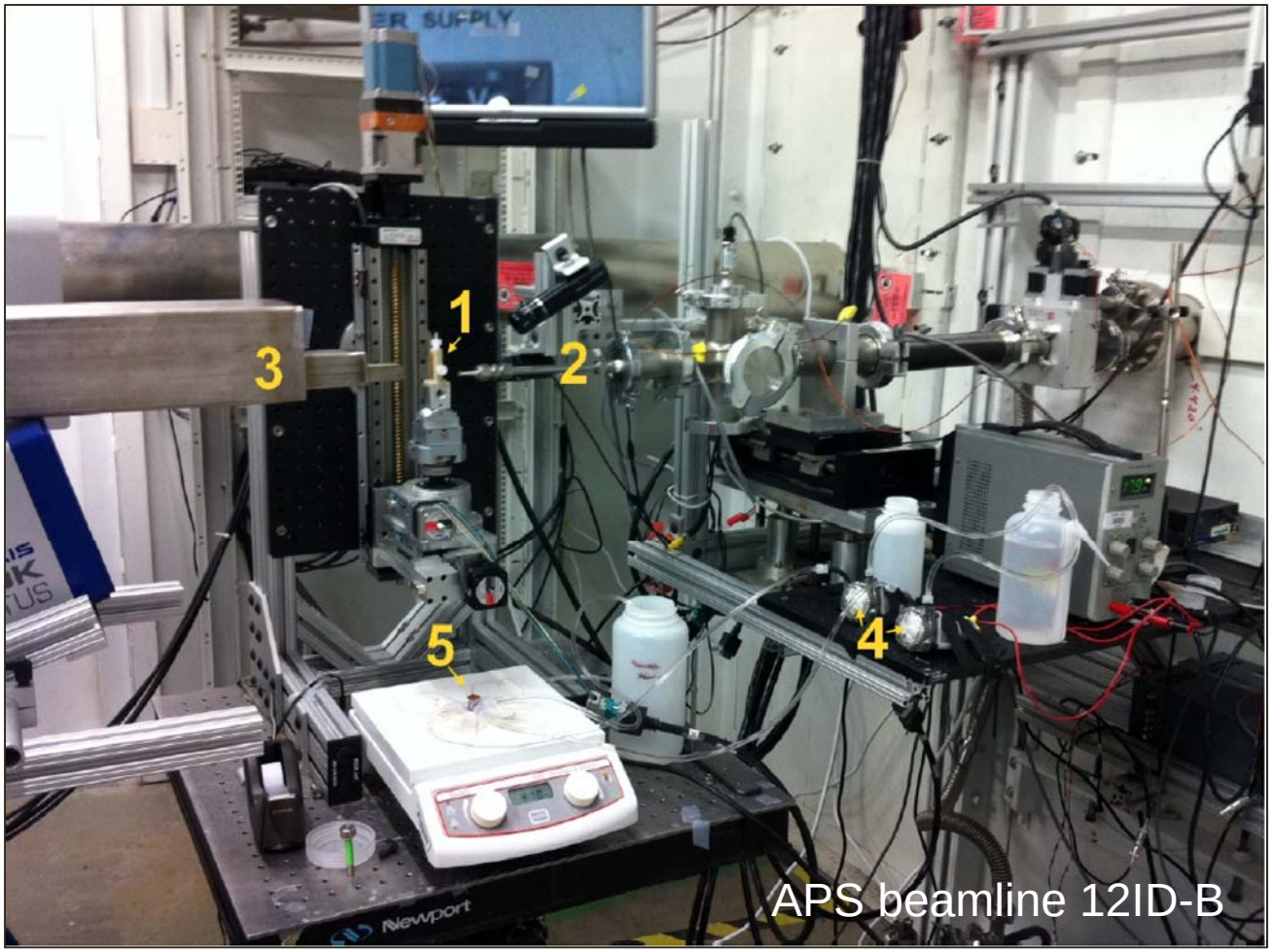


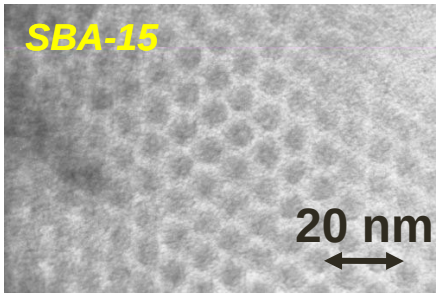
Experimental setup for the GISAXS experiments.

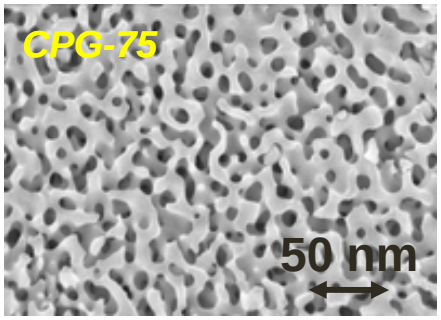
(1) In situ flow through cell. The substrate is placed in horizontal.
(2) Vacuum tube bringing the incident X-ray beam to the sample.
(3) Vacuum tube though which scattered X-rays are directed to the detector (far left).
(4) Peristaltic pumps used to pump $CaCl_2$ and $NaHCO_3$ solutions to the mixing cell.
(5) Mixing cell where the two solutions are mixed before being injected to the cell.

Synergistic NCGC Research (ORNL, LBNL-MSD, LBNL-ESD)

Mesoporous silica

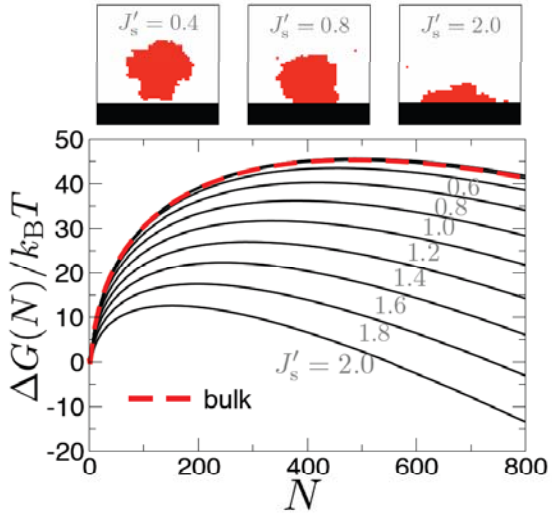
Tunable pore size; 2 – 100 nm

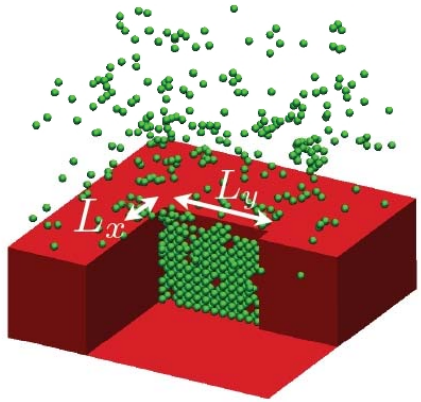
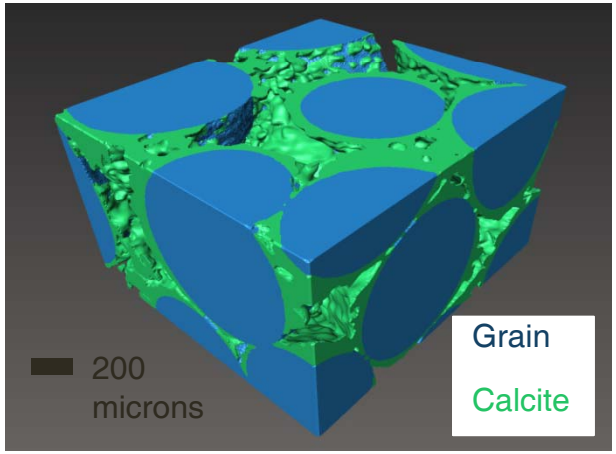
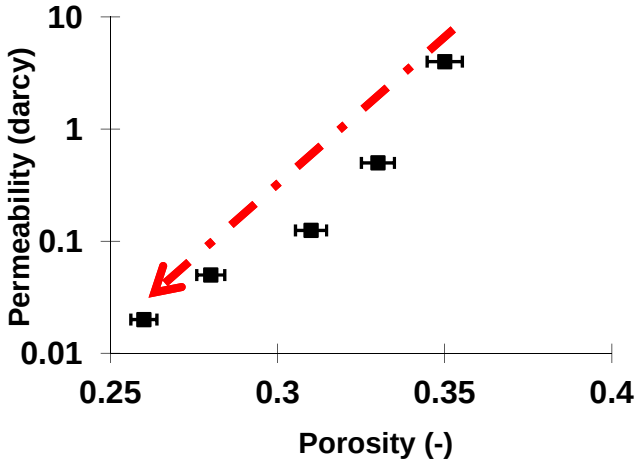




Neutron scattering experiments show that nucleation in nanopores is inhibited, probably due to kinetic effects (transport, solvent structure)

Statistical mechanics models





MicroCT at ALS BL 8.3.2