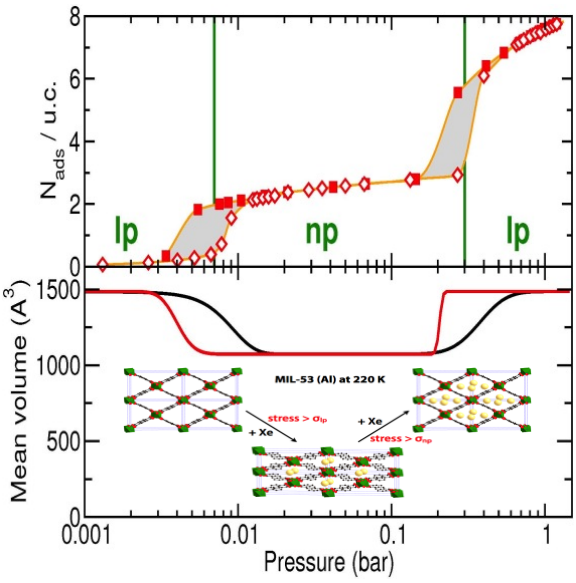
Breathing Solids: from Human Hair to Designer Nanoporous Materials

Alexander V. Neimark

Department of Chemical and Biochemical Engineering,
Rutgers University, 98 Brett Road, Piscataway, New Jersey 08854-8058, USA
Email: aneimark@rutgers.edu; Web: http://sol.rutgers.edu/~aneimark/

Phenomenon of adsorption-induced deformation attracted recently a considerable attention owing to its relevance to practical problems of mechanical stability and integrity of novel nanoporous materials and their adsorption properties. Guest molecules adsorbed in nanopores cause a substantial stress in the host matrix leading to its contraction or swelling depending on the specifics of host-guest interactions. Although various experimental manifestations of adsorption-induced deformation have been known for a long time since Leonardo da Vinci's studies of water sorption on human hair, a rigorous theoretical description of this phenomenon is lacking. I will present a general thermodynamic approach to predicting adsorption stress and respective deformation in various microporous and mesoporous materials based on molecular models of adsorption within elastic nanoscale confinements. Examples include carbons, zeolites, mesoporous crystals, and metal-organic frameworks.



A special attention will be paid to the enigmatic phenomenon of breathing of metal-organic frameworks in the course of gas adsorption-desorption cycles illustrated in the figure. Upon gas consumption, the crystal first contacts exhibiting a counter-intuitive abnormal "inhaling" transition from large pore (**lp**) phase to narrow pore (**np**) phase, and then expands back to **lp** phase that is associated with normal "inhaling". On the desorption pass, the reverse normal **lp**-**np** and abnormal **np**-**lp** "exhaling" transitions take place with a prominent hysteresis.

As a topical practical application, I will also discuss the deformation of coal during CO_2 sequestration at geological conditions.