Thermodynamics and Molecular Simulation of Adsorption-Induced Deformation of Nanoporous Materials

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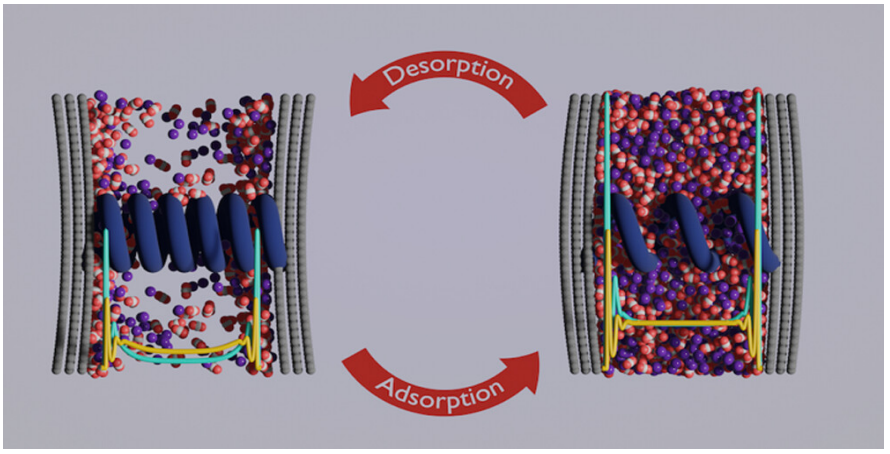
Guest molecules adsorbed in pores of a solid body exert substantial stress on the host matrix that causes its swelling or contraction depending on the nature of host-guest interactions. This phenomenon of adsorption-induced deformation has been known for a long time since Leonardo da Vinci's studies of water sorption on human hair. Various manifestations of adsorption-induced deformation are currently actively explored with respect to the design of novel nanoporous adsorbents and membranes for hydrocarbon separation, actuators, nanobumpers, energy storage devices, as well as the enhancement of gas recovery from shales and carbon dioxide sequestration in coal mines. Despite of the evident importance of the deformation effects during adsorption-desorption cycles, a rigorous theoretical description of this phenomenon is lacking. A similar problem arises in case of intrusion-extrusion of nonwetting fluids, the process involving high applied pressures. I will present a general thermodynamic approach to predicting adsorption stress and respective deformation in nanoporous materials of different origin based on molecular models of fluid sorption within elastic nanoscale confinements. The theoretical modeling is complemented by direct molecular simulation of adsorption-induced deformation using hybrid MD-MC methods. A special attention will be paid to the peculiar counterintuitive effects of non-monotonic deformation of a porous body upon fluid saturation with consequent stages of contraction and expansion. Most prominent is a so-called "breathing" behavior of MOFs during gas adsorption-desorption cycles. Unlike most materials that expand/swell on sorption (akin to inhaling) and contract on desorption (akin to exhaling), some microporous solids undergo atypical "inhaling/exhaling" transitions, contracting upon adsorption and expanding upon release. These transitions are associated with the adsorption induced phase transformation of the pore framework. Examples of comparison of the theoretical predictions with experiments include metal-organic frameworks (MOFs), microporous carbons and zeolites, mesoporous crystals, coal, and hierarchical micro-mesoporous monoliths.



Venerdì 21 giugno - ore 9:30
Aula Videoconferenze, DIMA -
Via Eudossiana 18, Roma
Link Google Meet: meet.google.com/ygy-egvf-bpo

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