Revealing Mechanisms of Adsorption-Induced Deformation by Molecular Simulations

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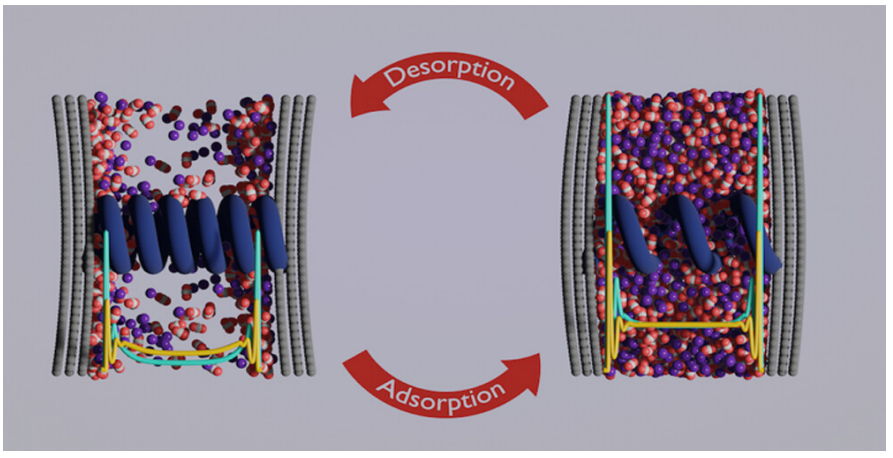
Guest molecules adsorbed in pores of a solid body exert substantial stress on the host matrix that causes its swelling or contraction depending on the nature of host-guest interactions. Various manifestations of adsorption-induced deformation are currently actively explored with respect to the design 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. Using iterative hybrid Monte Carlo and molecular dynamics simulations, we find that thermal fluctuations and flexibility of the host framework affect adsorption of guest molecules, and the deformation of loaded adsorbents occurs in a counterintuitive manner. Contrary to the expected gradual swelling during adsorption, adsorbent deformation is non-monotonic, it is characterized by contraction at low loadings, followed by partial expansion upon the pore filling. During the pore-filling process, guest molecules engender softening of the host structure to, in some cases, a nearly 100% increase in compressibility. However, upon the pore filling and further densification of the adsorbed phase, the structure hardens and compressibility decreases. As characteristic examples, we consider practical examples of metal-organic frameworks, microporous carbons, and shale organic matter [1,2].

1. Shivam Parashar, Nicholas J. Corrente, and Alexander V. Neimark, -Unveiling Non-Monotonic Deformation of Flexible MOFs during Gas Adsorption: From Contraction and Softening to Expansion and Hardening, Journal of Colloid and Interface Science, 2025, V.606, P. 88-95; DOI: 10.1016/j.jcis.2025.01.228.
2. Nicholas J. Corrente, Shivam Parashar, Raleigh Gough, Elizabeth L. Hinks, Peter I. Ravikovitch, and Alexander V. Neimark, -Modeling Structural Flexibility in 3D Carbon Models: A Hybrid MC/MD Approach to Adsorption-Induced Deformation, Carbon, 2025, V.230, 120160; DOI: 10.1016/j.carbon.2025.120160.



Giovedì 29 Maggio - ore 14:00
Aula Videoconferenze, DIMA -
Via Eudossiana 18, Roma
Link Google Meet: meet.google.com/nhz-keue-noe

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