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Adsorption-Induced Conformational Changes in Porous Materials MATTHEW CONNOLLY, CARLOS WEXLER, University of Missouri — In physisorption it is normally assumed that the adsorbent is structurally inert, its porous conformation unchanged by the adsorption; this assumption underlies most conceptual/theoretical framework used for characterization of porous solids. Recently, the mechanical response of the material has come under scrutiny: when a gas enters pores with sizes comparable with the range of the van der Walls forces an excess pressure/tension is created. Here we present a theoretical, computational and experimental demonstration of conformational expansion (breathing) of graphene-like adsorbents upon adsorption: Molecular dynamics simulations show the potential for supercritical hydrogen to open new pores in carbons. Grand Canonical Monte Carlo perturbative calculations demonstrate a reduction of the free energy of strip-shaped pores with gas loading upon a conformational change that increases the net size of micropores. Experimentally, reversible pore expansion during adsorption was measured by x-ray scattering for graphene oxide frameworks. These breathing modes have significant consequences for medium- to high-pressure adsorption, with modified adsorption isotherms that may require re-interpretation of standard models. Supported by DOE DE-FG02-07ER46411, ACS-PRF 52696-ND5, and NSF 1069091.

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