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Adsorption-induced breathing in nanoporous carbon[1] MATTHEW CONNOLLY, CARLOS WEXLER, University of Missouri — In most adsorption studies it is assumed that the adsorbent conformation is not changed by the adsorption; this assumption underlies most conceptual and theoretical framework used for characterization of porous materials and of adsorption in general. Recently, the behavior of the solid has come under review: when a gas enters pores with sizes comparable with the range of the van der Walls forces an excess pressure or tension exists. Here we present a theoretical, computational and experimental demonstration of breathing (expansion) of graphene-like adsorbents (graphene oxide frameworks, GOFs): 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 GOFs. These breathing modes have significant consequences for medium- to high-pressure adsorption, with modified adsorption isotherms that may require re-interpretation of standard models.

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Carlos Wexler
University of Missouri

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