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Gas adsorption studied by in situ powder diffraction: from structural evolution to thermodynamics

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In this presentation I will show examples of using in situ powder diffraction to simultaneously access the structure and adsorption properties of a small pore crystalline solid. (Quasi)-equilibrium isotherms and isobars can be built directly from sequential Rietveld refinements, both on adsorption and desorption, thus addressing the hysteresis and kinetics of gas adsorption/desorption. Detailed picture of guest reorganization with an increasing uptake can be obtained.
We investigated gas sorption in the porous γ-Mg(BH4)2 using neutron powder diffraction to accurately localize the guests and synchrotron X-ray powder diffraction to collect data along the adsorption isobars. The latter allows to study structural changes with pressure and temperature variation, giving insight into guest-host and guest-guest interactions, as well as to extract relevant thermodynamic parameters. I will discuss the intermolecular interactions, size effects and the role of hydridic hydrogen in physisorption. In this small-pore system, the effect of the probe size on the loading capacity and the location of the guest molecules is remarkable. While typically each pore can be occupied by one or two larger guests, the amount of hydrogen can go up to 5 molecules per pore, yielding the total capacity of 2.33 H2 molecules per Mg atom.

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