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Dense packing of molecular hydrogen in a porous hydride and the value of in situ diffraction studies of gas adsorption

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Nanoporous materials have attracted great attention for gas storage, however, high volumetric storage capacity remains still a challenge. We investigate [1] a magnesium borohydride framework with small pores and a unique partially negatively-charged non-flat interior for hydrogen and nitrogen uptake by using neutron powder diffraction, volumetric gas adsorption, inelastic neutron scattering, and first-principles calculations. Hydrogen and nitrogen occupy distinctly different adsorption sites in the pores with very different limiting capacities: 2.33 H2 and 0.66 N2 per Mg(BH4)2. Molecular hydrogen is packed extremely dense with about twice the density of liquid hydrogen (144 g H2/L of pore volume), independently measured by three experimental methods. A penta-dihydrogen cluster is discovered where H2 molecules in one position have rotational freedom whereas in another have a well-defined orientation and a directional interaction with the framework. This study [1] reveals that densely packed hydrogen can be stabilized in small-pore materials at ambient pressures.

Studies of physisorbed hydrogen require the use of neutron powder diffraction. For heavier molecules, in situ X-ray powder diffraction allows to study adsorption thermodynamics and kinetics [2, 3], revealing simultaneously the microscopic origins of guest-host and guest-guest interactions. (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.

[1] H. Oh, ⋯, Y. Filinchuk, Small-pore hydridic frameworks store densely packed hydrogen. Nature Chem., 2024, DOI: https://doi.org/10.1038/s41557-024-01443-x

[2] I. Dovgaliuk, V. Dyadkin, M. Vander Donckt, Y. Filinchuk, D. Chernyshov, ACS Appl. Mater. Interfaces 12, 2020, 7710.

[3] I. Dovgaliuk, I. Senkovska, X. Li, V. Dyadkin, Y. Filinchuk, D. Chernyshov, Angew. Chem. Int. Ed., 60, 2021, 5250.

Author: FILINCHUK, Yaroslav (Université catholique de Louvain)

Presenter: FILINCHUK, Yaroslav (Université catholique de Louvain)