Poster Presentation

MS99.P01

Unprecedented adsorption of molecular hydrogen in the porous hydride framework

Y. Filinchuk[1], N. Tumanov[1], V. Ban[1], H. Oh[2], M. Hirscher[2], B. Richter[3], T. Jensen[3], M. Hudson[4], C. Brown[4], G. Iles[5], S. Jorgensen[6]

[1]Institute of Condensed Matter and Nanosciences, Université Catolique de Louvain, Louvain-la-Neuve, Belgium, [2]Max Planck Institute for intelligent systems, Stuttgart, Germany, [3]Center for Materials Crystallography, Interdisciplinary Nanoscience Center and Department of Chemistry, Aarhus University, Aarhus, Denmark, [4]Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, MD, USA, [5]Department of Crystallography, Helmholtz-Zentrum Berlin, Berlin, Germany, [6]Chemical and Environmental Sciences Lab General Motors R&D Center, Warren, MI, USA

Recently the first porous hydride, gamma-Mg(BH4)2, featuring so-called "borohydride framework" and capable to store reversibly guest species was discovered [1]. This example clearly shows that the covalently bound hydride anions, such as borohydride, can act as directional ligands, capable to form molecular and polynuclear complexes, as well as framework structures typically occurring in classical coordination chemistry. Various small molecules are reversibly absorbed in gamma-Mg(BH4)2. In this work we show that molecular hydrogen and nitrogen have different adsorption sites in gamma-Mg(BH4)2, leading to different capacities on saturation and to different H2 and N2 BET areas. Only up to 0.66 N2 molecules are adsorbed per Mg atom, but the saturation capacity is double for the smaller hydrogen molecule. Moreover, at higher pressures, the second hydride phase forms with unprecedented hydrogen content of ~22 weight % (!). The density of hydrogen adsorbed into the pores is much higher than in liquid hydrogen, having no analogues among other porous systems. On the technical side, we will illustrate how in-situ diffraction at neutron and synchrotron sources allows to follow adsorption isobars, aiming for extraction of isosteric heats of adsorption directly from diffraction data, as well as for clarifying the microscopic mechanisms in terms of guest-host and guest-guest interactions.

[1] *Y. Filinchuk, B. Richter, T.R. Jensen, V. Dmitriev, D. Chernyshov, H. Hagemann, Angew. Chem. Int. Ed., 2011, 50, 11162-11166*

Keywords: porous materials, in-situ diffraction, hydrogen