Contribution ID: **151** Type: **Talk (20 min + 5 min discussion)**

Ultra-dense hydrogen stored in a metal hydride framework & investigated by Neutrons

Monday, 4 December 2023 13:40 (25 minutes)

Neutrons are a unique probe for non-destructive structural studies of energy materials, especially for the development of highly dense hydrogen stores. Thus, nano-porous materials have attracted great attention for gas storage, while the storage capacity still remains challenging. Here a magnesium borohydride framework with small pores was investigated 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. 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 reveals that densely packed hydrogen can be stabilized in small-pore materials at ambient pressures.

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Session Classification: Structure Research

Track Classification: Structure Research