This study developed novel hydrides for hydrogen storage through a new synthesis technique utilizing high hydrogen overpressure at elevated temperatures denoted as Molten State Processing, MSP. The MSP process was developed and used to modify and form new complex hydride compounds with desired characteristics. This synthesis technique holds the potential of fusing different known complex hydrides at elevated temperatures and pressures to form new complexes having different sorption and thermodynamic properties. The new complex hydrides produced by this method were identified through structural determination and thermodynamic characterization. Other possible high capacity hydrides are also investigated.

O-073  **Alane AlH$_3$ for Hydrogen Storage.**  V. A. Yartys,$^1$ J. P. Maehlen,$^1$ R. V. Denys,$^1$ M. Fichtner,$^2$ Ch. Frommen,$^2$ B. M. Bulychev,$^3$ H. Emerich,$^4$ Y. E. Filinchuk,$^5$ – Institute for Energy Technology, Kjeller, Norway; $^1$Institute of Nanotechnology, Research Centre Karlsruhe, Germany; $^3$Lomonosov Moscow State University, Moscow, Russia; $^4$Swiss-Norwegian Beam Line, European Synchrotron Research Facility, Grenoble, France

Alane AlH$_3$ combines high gravimetric and volumetric densities of hydrogen, making the goal of building a total H storage system with efficiency exceeding 5 wt.% H reachable. AlH$_3$ forms several polymorphic modifications, from which we have focused our studies on α- and γ-AlH$_3$. A significant decrease in hydrogen packing density, by 11 %, from 2.09$LH_2$ for the rhombohedral α-AlH$_3$ with corner-sharing AlH$_6$ octahedra; sp.gr. $R\overline{3}c$; a=4.44994(5); c=11.8200(2) Å to 1.85$LH_2$ for the orthorhombic γ-AlH$_3$ with both corner- and edge-sharing AlH$_6$ units thus containing double bridge bonds between Al and H; sp.gr. Pnnm; a=5.3803(1); b=7.3572(2); c=5.77526(5) Å was found by SR XRD and is caused by a formation of rather large cavities in γ-AlH$_3$. This results in a decrease of its stability compared to α-AlH$_3$. Studies of the kinetics and mechanism of the decomposition of α-AlH$_3$ and γ-AlH$_3$ performed by in situ SR XRD and thermal desorption spectroscopy studies show a higher activation energy of hydrogen desorption from α-AlH$_3$ compared to the γ-hydride (136 kJ/mol and 92 kJ/mol, respectively). Complex, double-peak, decomposition behaviour was observed for both modifications. For the γ-modification, following temperature increase, three overlapping events were observed between 80 and 120 °C; γ→α transformation and two thermal decomposition processes, for γ- and for α-alane. Decomposition AlH$_3$ → Al + 3/2 H$_2$, which releases 10 wt.% H, because of small decomposition enthalpy and low desorption temperatures, makes AlH$_3$ very attractive material for the on-board hydrogen storage applications. This work has received a support from INTAS project 05-1000005-7665 “New Alane: Novel Reversible Hydrogen Storage Materials Based on the Alloys of Al”.

O-074  **H$_2$ Physisorption in Carbons and Metal Organic Frameworks.**  C. C. Ahn, – California Institute of Technology, Pasadena, CA, USA

High surface area physisorbers are typically capable of storing 4 to 5 wt.% of hydrogen at 77K. In the case of carbons, including activated carbons and aerogels, we can expect the surface excess adsorption saturation value to follow the linear behavior noted by Chahine of 1 wt% gravimetric density for every 500 m$^2$/gm. The saturation point generally occurs at pressures of 20 to 40 bar. In metal organic frameworks that have surface areas of ~3000m$^2$/gm, we note, presumably due to the high molecular weight vertices of these structures, deviations from the linear behavior that is seen in carbons toward lower gravimetric density. We also note that the low-pressure isotherm behavior to 1 bar pressure, while useful for determining the Henry’s law constant, is inadequate in assessing the ultimate surface excess quantity of sorbent. The typical “heat” we measure is derived from a Henry’s law analysis, and yields a zero coverage differential enthalpy of adsorption in the range of 4 to 8 kJ/mole for most physisorbents. For practical applications, however, the isosteric enthalpy of adsorption is the more useful quantity for engineering applications as it typically shows a decrease in the heats measured as a function of gravimetric density, of importance in determining the heat transfer requirements of a storage tank.

O-075  **Hydrogen Adsorption in Metal-Organic Frameworks.**  M. Hirscher, B. Panella, – Max-Planck-Institut für Metallforschung, Stuttgart, Germany

Hydrogen can be reversibly stored by adsorption on microporous materials with high specific surface areas at liquid nitrogen temperature. Recently, special attention has been given to metal-organic frameworks (MOFs), which possess the lowest densities of all known crystalline materials. These coordination polymers consist of metal oxide clusters connected by rigid aromatic linkers giving a three dimensional porous structure. We present new hydrogen adsorption measurements for MOFs, which have been prepared by large-scale synthesis methods. The results will be compared with hydrogen uptake measurements of other microporous materials, e.g., carbon nanostructures, zeolites etc. For the saturation value of hydrogen uptake an almost linear correlation with the specific surface area is found for all materials, whereas, the adsorption at lower pressures depends on the pore size or the metal ions. This will be shown by comparing various MOFs possessing different central-metal ions and organic ligands.

O-076  **Organometallic Compounds with Very Large Pore Volumes as Hydrogen Storage Materials.**  M. Latroche,$^1$ S. Surbé,$^2$ C. Serre,$^3$ F. Millange,$^4$ G. Férey,$^4$ – Laboratoire de Chimie Métallurgique des Terres Rares, CNRS, Thiais, France; $^1$Institut Lavoisier, Université de Versailles, Versailles, France

This work deals with microporous materials able to store reversibly hydrogen gas. Combining targeted chemistry and computational design, different porous metal (Al, Cr) terephthalate and benzenedicarboxylate have been obtained with very large pore sizes and giant surface areas [1]. Beside the usual properties of these porous compounds, those zeotype cubic structures have potential properties for hydrogen storage. For example, MIL-101 [2] exhibits at liquid nitrogen temperature a capacity of 4.5 wt.%, one of the largest value ever reported for Metal Organic Framework (MOF) materials. Significant hydrogen uptake are also observed at room temperature (about 0.4wt.%) though the reversible capacities are still to be improved. [1] G. Ferey, C. Mellot-Draznieks, C. Serre,