

# Project Report



**Application No.** 2003

**Short title** Hydrogen storage measurements in oxidized and metal decorated single-wall carbon nanohorns

## **Objectives: short, medium and long term (<250 words)**

The hydrogen storage properties of various forms of carbon - carbon nanotubes, fullerene, graphene etc - have been widely studied using experimental approaches often combined with theoretical calculations. However, their H<sub>2</sub> storage capacity and overall performance are quite low especially at room temperature due to weak van der Walls interactions between H<sub>2</sub> molecules and the surface of the carbonaceous matrix. Several studies have shown that the interaction of hydrogen with single-wall carbon nanohorns (SWNHs) is far stronger than in the case of carbon nanotubes, and as such they have been considered quite appealing as possible hydrogen storage materials. Our group has studied the effects of confining molecular hydrogen within SWNHs. High-resolution quasi-elastic and inelastic neutron spectroscopies at low temperatures (quite below room-temperature) have been carried out to characterize the confinement effects as well as study its temperature dependence. The results have shown that hydrogen interacts far more strongly with the SWNHs than it does with carbon nanotubes, suggesting that nanohorns and related nanostructures may offer significantly better prospects as lightweight media for hydrogen storage applications. For a more complete characterization of the hydrogen storage properties, it was necessary to perform a systematic series of H<sub>2</sub> adsorption/desorption measurements (volumetric but also gravimetric) at different temperature and pressure conditions; such experiments were carried out in HYSORB laboratory.

## **Brief summary of work carried out:**

The samples received (as synthesized and undoped) were investigated with regard to their structural / morphological properties as well as their H<sub>2</sub> sorption performance at different temperatures (77 K, 298 K) and pressures (1-120 bar). Different methods (FTIR, TGA, XRPD, SEM) were used for the typical characterisation. On the other hand N<sub>2</sub> adsorption –desorption isotherms obtained at 77 K were of type II (based on IUPAC classification) and revealed moderate surface area (around 250 m<sup>2</sup>/g) and pore volume (around 1 cm<sup>3</sup>/g) values. The hydrogen storage capacity of the materials was determined at 77 and 298 K up to 120 bar, using both gravimetric (RUBOTHERM balance) and volumetric (PCTPro-2000) setups as well as ultrapure (99.9999 %) hydrogen gas. In all cases a small amount (~130 mg) of each sample was placed in a stainless steel sample cell closed with a metal seal and had to be degassed under high vacuum (1.E-06 mbar) at 523 K for at least 24 h. Volume calibrations with helium gas were performed prior to each measurement using inert non-absorbing samples having the same skeletal volume with the carbon materials examined. Overall the carbon samples showed very low hydrogen uptake (less than 0.1 wt%) at room temperature that increased practically linearly with pressure (Henry-like behaviour), while no hysteresis was observed during desorption.

## **Main achievements intended for publication <250 words**

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**Further comments:** No