HYDROGEN ADSORPTION ON PARTIALLY OXIDISED MICROPOROUS CARBONS.

J.B. Parra[1], C.J. Durân-Valle[2], C.O. Ania[1], M.L. Sânchez[3], C. Otero Areân[4]

(1) Instituto Nacional del Carbdn, C.S.I.C., Apartado 73, 33080 Oviedo (Spain)

(2) Departamento de Quimica Inorgknica, Universidad de Extremadura, 06071 Badajoz (Spain)

(3) Departamento de Quimica-Fisica, Universidad de Extremadura, 06071 Badajoz (Spain)

(4) Departamento de Quimica, Universidad de las Islas Baleares, 07122 Palma de Mallorca (Spain)

The search for cost effective adsorbents for large scale gas separation, storage and transport constitutes a present day strategic issue in the energy sector, propelled mainly by the potential use of hydrogen as an energy vector in a sustainable (and cleaner) energy scenario. Both, activated carbons and carbon based nanostructured materials have been proposed as potential candidates for reversible hydrogen storage in cryogenically cooled vessels. For that purpose, surface modification so as to enhance the gas solid interaction energy is desirable. We report on hydrogen adsorption on microporous (active) carbons which have been partially oxidised with nitric acid and ammonium persulfate. From the corresponding hydrogen adsorption isotherms (Fig. 1) an isosteric heat of about 3 kJ mol^{-1} was derived. This value is in agreement with that of about 3 to 4 kJ mol^{-1} obtained by quantum chemical calculations on the interaction between the hydrogen molecule and simple model systems (Fig. 2) of both, hydroxyl and carboxyl groups. Further research is in progress with a view to further increases the gas solid interaction energy. However, the values so far obtained are significantly larger than the liquefaction enthalpy of hydrogen: 0.90 kJ mol^{-1}; and this is relevant to both, hydrogen separation from gas mixtures and cryogenic hydrogen storage.

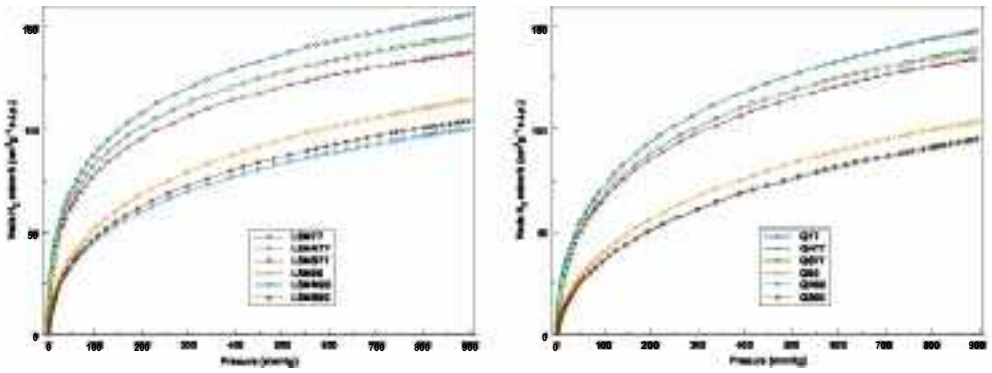

Fig. 1. Hydrogen adsorption isotherms on: (1) Activated carbons (LSM and Q); (2) the same samples after oxidation with HNO_3 (LSMN and QN) and with $(NH_4)_2S_2O_8$ (LSMS and QS). Numbers denote the adsorption temperature.

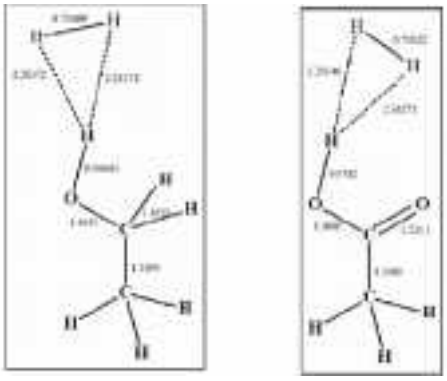

Fig 2. Proposed interaction schemes between a hydrogen molecule and oxygenated carbon surface functionalities: hydroxyl and carboxyl.