

Project C-10: Nanostructured carbons for hydrogen storage

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This new IEA project, brought into Task 17 in late 2003, seeks to explore the role of nanostructure on H₂ storage on carbons. Experimental (advanced structural characterization and measurement of H₂ isotherms) and theoretical (both *ab initio* calculation of potential H₂/carbon-surface/metal-catalyst interactions and reverse Monte-Carlo simulations of the carbon nanostructure) approaches will be adopted. Characterization data will provide a basis for the development of simulation of nanoporous carbon structures. SANS data has demonstrated that light gas interactions occur predominantly in the nano-dimensioned pores, i.e., < 3nm. The H₂ adsorption behavior of a broad selection of nanoporous carbons is being determined over the pressure range 0-20 bar and at ambient and liquid N₂ (77K) temperature utilizing an Intelligent Gravimetric Analyzer (IGA) system by Hiden Technologies. None of the samples tested to date have shown significant ambient temperature H₂ uptakes (typically < 0.2 wt% uptake). The greatest uptake at ambient temperature was ~0.3 wt% (wood based activated carbon). However, the same sample exhibited a H₂ uptake in excess of 8 wt% at 77K.

Ab initio calculations suggest that the presence of a metal catalyst on the carbon surface promotes the adsorption of hydrogen. These data suggest the combination of highly nanoporous activated carbon and a finely dispersed metal catalyst might offer the best chance for H₂ storage on carbon. Future work will focus on the experimental determination of the role of the metal catalyst in the interaction of H₂ on carbons. The influence of catalyst morphology on the interaction between C and H will be examined. Comparisons of pure and impure nanotubes and activated carbons and fibers with and without dispersed metal catalyst will allow insight into the role of the catalyst.