MAR07-2006-020177

Abstract for an Invited Paper
for the MAR07 Meeting of
the American Physical Society

Hydrogen Storage in Chemically Reducible Microporous Ti Oxides

DAVID ANTONELLI, University of Windsor

Micro- and mesoporous Ti oxides with controlled pore sizes from 12 Å to 26 Å were synthesized. The hydrogen storage capacity at 77 K was tested as a function of surface area, pore size, and reducing agent. Surprisingly, the oxidation state of the surface Ti species had a greater effect on the storage densities than surface area or pore size. The 12 Å material reduced with bis(toluene) Ti possesses a surface area of less than 500 m^2/g, but absorbs over 5 wt% and 40 kg/m^3 of H_2 reversibly at 77K and 100 atm. The H_2 binding enthalpies increased from less than 5 kJ/mol to over 8 kJ/mol as the surface oxidation state of the Ti decreased. The enthalpies also increased with surface coverage, which is opposite to all other cryogenic physisorption systems. These results suggest that a Kubas-type σ H_2 complex is involved and that further tuning of the H_2 binding enthalpies through use of various chemical reagents may achieve even higher storage levels at more moderate temperatures.