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Stable Room Temperature Hydrogen Storage in Titainum-Doped Silica. JASON SIMMONS, TANER YILDIRIM, NIST Center for Neutron Research, AHMAD HAMAED, DAVID ANTONELLI, Department of Chemistry and Biochemistry, University of Windsor — The optimum conditions for viable room temperature hydrogen storage require materials that possess isoteric heats of adsorption in between that of standard physisorbers and chemisorbers, typically in the ∼20-30 kJ/mol regime. It has been theoretically predicted that transition metal atoms incorporated onto high surface area materials could enable significant room temperature storage; herein we demonstrate a possible experimental proof of these predictions. Titanium(III) complexes are grafted onto porous silica hosts, then activated to generate sites for dissociative adsorption of hydrogen gas. Using a combination of sorption measurements and inelastic neutron scattering, we show that the activated titanium provides strong hydrogen binding sites at room temperature and that adsorbed hydrogen is stable for long periods of time at ambient conditions. Further, the hydrogen can be desorbed under mild processing conditions. Neutron vibrational spectra agree well with theoretically predicted vibrational modes of the Ti—H complex. These results represent an important step towards reversible room temperature hydrogen storage.

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