Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Towards 9 weight percent, reversible, room temperature hydrogen adsorbents: Hydrogen saturated organometallic bucky balls YUFENG ZHAO, YONG-HYUN KIM, A. C. DILLON, M.J. HEBEN, S. B. ZHANG, National Renewable Energy Laboratory — A new concept for high-capacity hydrogen absorbents is introduced by first-principles calculations. Transition metal (TM) atoms bound to fullerenes are proposed as a medium for high density, room temperature, ambient pressure storage of hydrogen. TMs bind to C60 or C48B12 by charge transfer interactions to produce stable organometallic bucky balls (OBBs) and bind to multiple dihydrogen molecules through the so-called Kubas interaction [1]. A particular scandium OBB can bind as many as eleven hydrogen atoms per TM, ten of which are bound in the form of dihydrogen molecular ligands that can be adsorbed and desorbed reversibly. In this case, the calculated binding energy is around 0.3 eV/H2, which is ideal for use on-board vehicles. The theoretical maximum retrievable H2 storage density is about 9 weight percent. This work was supported by the U.S. DOE EERE, BES/MS, and BES/CS under contract No. DEAC36-99GO10337.
[1] G.J. Kubas, J. Organometallic Chem. 635, 37 (2001).

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Date submitted: 29 Nov 2004 Electronic form version 1.4