Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Thermodynamic and kinetic destabilization in $LiBH_4$-based hydride systems JOHN VAJO, WEN LI, PING LIU, HRL Laboratories, LLC — The $LiBH_4/MgH_2$ destabilized hydride system has attracted considerable attention recently because it is a reversible system, based on the $[BH_4]^-$ anion, with a high hydrogen capacity (11.6 wt % gravimetric). However, hydrogen release during a temperature ramp occurs in two steps with dehydrogenation of MgH_2 to Mg + H_2 occurring first followed by reaction of Mg with $LiBH_4$ to form LiH + MgB_2 + H_2. These two steps occur despite there being a direct reaction that is thermodynamically allowed at lower temperatures. In this talk we describe a $LiBH_4$-based hydride system that is kinetically as well as thermodynamically destabilized. In this system, a direct (concerted) dehydrogenation reaction of $LiBH_4$ occurs at temperatures lower than the dehydrogenation temperature of any of the components separately. In addition, the system is reversible with an equilibrium hydrogen pressure (based on preliminary measurements) that is ~20X higher than the pressure for the $LiBH_4/MgH_2$ system.

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Date submitted: 11 Nov 2008

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