

## REVERSIBLE HYDROGENATION OF $MgB_2$ TO $Mg(BH_4)_2$

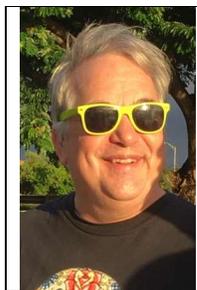
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Among the many complex hydrides that have been explored as hydrogen carriers, magnesium borohydride,  $Mg(BH_4)_2$ , has been found to possess the best combination of properties for utilization as a reversible hydrogen storage medium including a gravimetric H density of 14.9 wt% H and favourable thermodynamics for the dehydrogenation of  $Mg(BH_4)_2$  to  $MgB_2$  ( $\Delta H = 39$  kJ/mol H,  $\Delta S = 112$  J/K mol H). However, due to extremely slow kinetics, hydrogen cycling has been accomplished for this system only at extreme conditions (400 °C, 900 atm). Less extensive, reversible dehydrogenation has been accomplished at <200 °C. We have found that the coordination of selected Lewis bases enhances the kinetics and shifts the product selective from  $Mg(B_3H_8)_2$  to  $Mg(B_{10}H_{10})$  representing a change in the maximum hydrogen release from 2.7 to 8.1 wt %. These findings prompted an investigation of the effects Lewis base on the more extensive hydrogen cycling between  $MgB_2$  and  $Mg(BH_4)_2$  which has revealed that mechanical milling of  $MgB_2$  with additives including THF and graphene results in a pronounced kinetic enhancement. XRD,  $^{11}B$  NMR, and FTIR analysis indicate that this treatment does not result in a bulk: chemical transformation; formation of an adduct; or phase transition. However, variable temperature, high pressure  $^1H$  NMR studies indicate that the modified material does contain sites in which the binding energy of physi-sorbed  $H_2$  is increased above the <3 kJ/mol value found for un-treated  $MgB_2$  to ~ 6 kJ/mol. The resulting increase in the residence of absorbed  $H_2$  may at least partially account for the improvement in the overall kinetics we have observed for the hydrogenation of the boride to borohydride. This hypothesis and the possible nature of the  $H_2$  binding sites in the modified material will be discussed in context of our overall goal of developing a comprehensive model of reversible hydrogenation of  $MgB_2$  to  $Mg(BH_4)_2$ .



Dr. Craig Jensen is a full professor in the Department of Chemistry of the University of Hawaii. He has authored or co-authored 156 peer-reviewed publications and 10 U.S. patents. Prof. Jensen was named the U.S. Department of Energy Hydrogen program's "1999 Research Success Story" and presented with their "R&D" award in 2004. He was a co-chairman of the 2006 International Symposium on Metal-Hydrogen Systems and the 2007 Hydrogen-Metal Systems Gordon Research Conference. In 2003, Dr. Jensen founded Hawaii Hydrogen Carriers, LLC and has since served as the company president.