**OBJECTIVE AND SIGNIFICANCE:** The objective of this project is to obtain key information that can be used for the development of a comprehensive, multi-scale computational model of reversible hydrogenation of magnesium boride, MgB$_2$ to magnesium borohydride, Mg(BH$_4$)$_2$. If successful, the project will significantly accelerate the discovery of boride materials for practical hydrogen storage applications. The project provides excellent training on state-of-the-art instrumentation to the participating UH graduate students, postdoc fellows, and early career scientists and enhances research competitiveness at UH by strengthening ties with U.S. national laboratories.

**BACKGROUND:** The magnesium boride/magnesium borohydride (MgB$_2$/Mg(BH$_4$)$_2$) material system is one of the few cyclable materials that has a demonstrated gravimetric hydrogen storage capacity greater than 11 wt% and hence has a potential to be utilized in a hydrogen storage system that meets U.S. DOE hydrogen storage targets. This project works towards obtaining experimental information of 1) the bulk, nano-scale, and meso-scale structural changes occurring at elevated pressure following mechano-chemical modification of MgB$_2$; 2) the reaction pathway of the reversible hydrogenation of MgB$_2$ to Mg(BH$_4$)$_2$; 3) the effect of elevated pressure and mechano-chemical modification on the chemical reaction pathways; 4) the interactions at solid-gas interfaces and particle surfaces; and 5) the kinetics and thermodynamic parameters associated with each step of the hydrogenation reaction pathway. The fundamental experimental information derived from the project will be used for the development of a comprehensive, multi-scale computational model of reversible hydrogenation of MgB$_2$ to Mg(BH$_4$)$_2$ at the Lawrence Livermore National Laboratory.

This EPSCoR project is a collaborative effort between UH (HNEI, Mechanical Engineering (ME), Department of Chemistry, and Hawai‘i Institute of Geophysics (HIGP)) and the National Renewable Energy Laboratory (NREL). The HNEI effort is focused on Vibrational and Raman Spectroscopy studies of modified MgB$_2$, as well as Calorimetry studies of the initial stages of hydrogen uptake.

**PROJECT STATUS/RESULTS:** We have prepared ball milled samples of pure magnesium boride and MgB$_2$ containing various modifiers, and performed *in-situ* hydrogenation studies of the samples using Diffuse Reflectance Infrared Transform Spectroscopy (DRIFTS) in collaboration NREL. The purpose of the DRIFTS studies is to provide insights into the initial steps involved in the hydrogenation of modified MgB$_2$ materials. We are also probing the presence of B-H, Mg-H, and unanticipated bonding in the hydrogenated materials. The DRIFTS spectra of the modified MgB$_2$ samples indicate two unique overlapping vibrational peaks in the 1200-1400 cm$^{-1}$ region, that increase in intensity with hydrogenation temperature (Figure 1). These new broad peaks can be observed to varying degrees in the modified samples between 180-350 °C, hence are attributed to hydrogen interaction with the MgB$_2$. Comparison of the relative intensities of the 1200-1400 cm$^{-1}$ features suggest that the anthracene and Mg-THF additives lead to the highest surface hydrogen uptake at these low hydrogen pressure conditions. We are currently ascertaining whether the vibrational peaks observed at 1200-1400 cm$^{-1}$ are due to B-H-B bond formation during the initial stages of hydrogen uptake. Furthermore, Raman studies are underway to assist in correlating the changes in boron-boron bonding occurring following mechano-chemical modification of MgB$_2$, to the extent of hydrogen uptake.

![B-H Bend Region](image)

Figure 1. Summary DRIFTS spectra of modified MgB$_2$ materials in the B-H bend region showing presence of new peak at 1200-1400 cm$^{-1}$ during hydrogenation.

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