Announcement

An oral examination in defense of the dissertation for the degree
Doctor of Philosophy in Physics

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M.S. in Physics, May, 2013, University of Missouri – St. Louis
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DFT INVESTIGATIONS OF HYDROGEN STORAGE MATERIALS

Date: March 25, 2016
Time: 2:30 p.m. to 3:30 p.m.
Place: M101 Center for Nano Science

Abstract

Hydrogen serves as a promising new energy source having no pollution and abundant on earth. However the most difficult problem of applying hydrogen is to store it effectively and safely, which is smartly resolved by attempting to keep hydrogen in some metal hydrides to reach a high hydrogen density in a safe way. There are several promising metal hydrides, the thermal dynamic and chemical properties of which are to be investigated in this dissertation. Sodium alanate (NaAlH4) is one of the promising metal hydrides with high hydrogen storage capacity around 7.4 wt. % and relatively low decomposition temperature of around 100 °C with proper catalyst. Sodium hydride is a product of the decomposition of NaAlH4 that may affect the dynamics of NaAlH4. The two materials with oxygen contamination such as OH- may influence the kinetics of the dehydriding/rehydriding processes. Thus the solid solubility of OH- groups (NaOH) in NaAlH4 and NaH is studied theoretically by DFT calculations. The thermal dynamic functions using phonon calculations in harmonic approximation were performed to plot the solid solution phase diagrams using grand canonical linear programing (GCLP) method.

Magnesium boride [Mg(BH4)2] is another promising hydrogen storage material with higher hydrogen capacity about 14.9 wt. % and the decomposition tempature of around 250 °C. Beyon all of the advantages, there is one flaw that restrains its application that is it may produce some polyboron compounds like MgB12H12 preventing from further release of hydrogen. Adding some transition metals that form magnesium transition metal ternary borohydride [MgaTMb(BH4)c] may skip the formation of stable polyboron compounds and simply the decomposition process to release hydrogen with generating only corresponding ternary borides (MgaTMbBc). The search for the probable ternary borides and the corresponding pseudo phase diagrams as well as the decomposition thermal dynamics are performed using DFT calculations and GCLP method to present some possible candidates.

Defense of Dissertation Committee

Eric H. Majzoub, Ph.D. (Chair)
Julia E. Medvedeva, Ph.D.
Yew San Hor, Ph.D.
Sonya Bahar, Ph.D.
Phillip B. Fraundorf, Ph.D.
Stephen M. Holmes, Ph.D.