VI.D.5 Metal Perhydrides for Hydrogen Storage

Jiann-Yang Hwang (Primary Contact), Shangzhao Shi, Stephen A. Hackney, Douglas J. Swenson, Zhiyong Xu
Michigan Technological University
1400 Townsend Drive, Houghton, Michigan 49931-1295
Phone: (906) 487-2600; Fax: (906) 487-2921; E-mail: jhwang@mtu.edu

DOE Technology Development Manager: Grace Ordaz
Phone: (202) 586-8350; Fax: (202) 586-9811; E-mail: Grace.Ordaz@ee.doe.gov

DOE Project Officer: Jim Alkire
Phone: (303) 275-4795; Fax: (303) 275-4753; E-mail: James.Alkire@go.doe.gov

Contract Number: DE-FG36-05GO15003

Start Date: April 1, 2005
Projected End Date: March 31, 2009

Objectives

Develop novel materials that

- have sufficiently high capacity for hydrogen storage,
- are able to liberate hydrogen in easy manner, and
- can be regenerated economically.

The novel materials we plan to develop in this project are termed metal perhydrides. In perhydride molecules, the metal atoms form chemical bonds with hydrogen clusters instead of individual hydrogen atoms.

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Storage section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

- A. Cost
- B. Weight and Volume
- C. Efficiency

Technical Targets

This project is conducting fundamental investigations of metal perhydrides. Insights gained from these investigations will be applied toward the design and synthesis of hydrogen storage materials that meet the DOE 2010 hydrogen storage targets of cost, weight and volume, and energy efficiency.

Approach

Conduct materials modeling

- Simulate the thermodynamics of metal perhydrides with established models
  - *ab initio* Hartree-Fock method
  - Density functional theory approach

  - Complete active space method
- Establish new models
  - Use molecular orbit theory
  - Analogize the bonding structures in hydrogen ion clusters to those in metal clusters
  - Analogize the bonding structures between metal atoms and hydrogen ion clusters to those between metal atoms and ligand groups

Identify and investigate the metal perhydrides

- Use microwave approach to ionize hydrogen under various conditions (especially atmospheric and above-atmospheric pressures)
- Investigate reactions of ionized hydrogen with metals and/or metal precursors
- Develop approaches for post-reaction treatment of the reaction products with pressurized hydrogen and/or at cryogenic temperatures
- Use in-situ identification of hydrogen ion clusters and perhydride species with Fourier transform infrared and hydrogen content analyzer
- Identify post-reaction of perhydride species with mass spectrometry, X-ray photoelectron spectroscopy, nuclear magnetic resonance spectroscopy, differential scanning calorimeter, thermogravimetric analysis**,** X-ray diffraction, scanning electron microscopy, and transmission electron microscopy

Accomplishments

This project is newly initiated and there are no accomplishments to report at present.