Metal Perhydrides for Hydrogen Storage

(Project ID#STP49)

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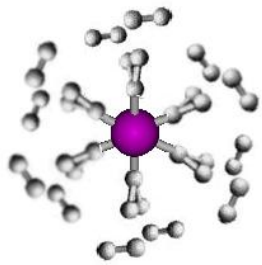
Objective

Develop novel materials that

- have sufficient high capacity for hydrogen storage
- are able to liberate hydrogen in easy manner
- can be regenerated economically

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



Technical Barriers

This project addresses primarily the following technical barriers from the hydrogen storage section of the Hydrogen, Fuel cells and Infrastructure Technologies Multi-Year Research, Development and Demonstration Plan: Planned program activities for 2003-2010, New Materials and Concepts Feasibility:

A. Cost

B. Weight and Volume

C. Efficiency

Approach

Materials modeling

- Simulate the thermodynamics of metal perhydrides with established models
  - *ab initio* Hartree-Fock (HF) method
  - Density Functional Theory (DFT) approach
  - Complete Active Space (CAS) 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 complex 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
- in-situ identification of hydrogen ion clusters and perhydride species with FTIR and hydrogen content analyzer
- post-reaction identification of perhydride species with Mass Spectometry (MS), X-ray photoelectron spectroscopy (XPS), Nuclear Magnetic Resonance Spectroscopy (NMR), Differential Scanning Calorimeter (DSC), Thermogravimetric Analysis (TGA), XRD, SEM, TEM

’05 Work Plan

Model the perhydrides structures and thermodynamics

- Simulate the thermodynamics of metal perhydrides with established models
  - calculate the formation energy
  - simulate the molecular structure of the metal perhydrides

    simulation will be performed on perhydrides of transition metals, light metals and metal complex Simulate the thermodynamics of metal perhydrides with established models
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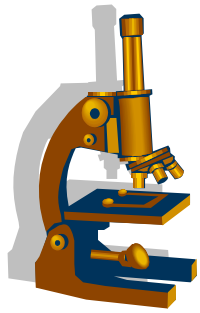
Investigate the conditions for ionization of hydrogen molecules and identify the formation of hydrogen ion clusters



- **Electromagnetic field intensity**
- **Carrier gases and flow-rate**
- **Hydrogen concentration**
- **Pressure (in vacuum range) & temperature**

Investigate the reactions of ionized hydrogen with metals and/or metal precursors and identify the formation of perhydride species

- **Transition metals**
- **Light metals**
- **Metal complex**

’06 Work Plan

Construct a reactor with enhanced functions for perhydride synthesis and identification

- Both in-situ FTIR & in-situ analysis of hydrogen content
- Capable of identification and analysis of gaseous, liquid and/or solid species during the process
- Capable of conducting reactions and/or post-reaction treatments of the reaction products under high (above atmospheric) pressures & at low (cryogenic) temperatures
- Capable of sampling reaction products under high pressures and/or at low temperatures for off-line characterizations

Develop approaches with enhanced functions for charcterization of perhydride species

- characterization of pressurized samples
- characterization of cryogenized samples

Advance the investigations performed in ’05 to high pressures and cryogenic temperateratures

- investigate the hydrogen ion species during high pressure hydrogen ionization
- investigate the perhydride formation in high pressure reactions of metals with hydrogen ion species
- investigate the effects of post-reaction treatment on the metal-hydrogen reaction products
  - under above atmospheric hydrogen pressures
  - at cryogenic temperatures