Overview

Timeline

- Start- Jan. 2005
- Finish- Sep. 2009
- 25% complete

Barriers

- Slow kinetics
- Low reversibility
- Release of undesired compounds

Budget

- Total project funding
  - DOE share: $720K
  - Contractor share: $180K
- Funding received in FY05: $150K
- Funding for FY06: $300K

Partners

- HRL labs – MgH₂ + Si, LiBH₄ + MgH₂
- Sandia National Labs- Li-Mg-N-H
- Other partners for future collaborations
Objectives

• Overall
  – Discover catalysts for metal hydride systems to achieve fast kinetics and high selectivity, thus to meet DOE’s 2010 targets for start time (4 s), flow rate (0.02 (g H₂/s)/kW) and refill time (3 min)

• 2005
  – Design, setup and validate combinatorial nano-synthesis systems
  – Design, setup and validate high throughput screening apparatus
  – Screen metal hydride candidates based on thermodynamic calculations

• 2006
  – Screen catalysts for MgH₂+Si system dehydrogenation and rehydrogenation
  – Screen catalysts for Li-Mg-N-H system dehydrogenation and rehydrogenation
  – Screen catalysts for LiBH₄+MgH₂ system dehydrogenation and rehydrogenation
Approach

Complex hydrides & catalysts design: Sandia, HRL, Intematix

Validation of leads: Sandia, HRL, Intematix

Combinatorial complex hydrides-catalysts development cycle

High throughput Screening: Intematix

Combinatorial Synthesis: Intematix
Approach

- **Metal hydrides preparation**
  - Study the chemical properties of metal hydride candidates
  - Design metal hydride synthesis process

- **Combinatorial catalysts preparation**
  - Design catalyst compositions
  - Design combinatorial nano-catalyst synthesis process

- **High throughput screening of catalysts**
  - Design high throughput methods for quick and qualitative screening
  - Collaborate with MHCoE partners for detailed characterization
  - Optimize catalyst compositions for further screening
Conducted Metal Hydride Candidates Evaluation

- Database search/calculations of ca. 200 candidate reactions using HSC Chemistry®
- Identified more than 15 reaction systems with > 6 wt% H₂ and P-T windows close to DOE targets
- Identified many potential reaction systems with high H₂ wt% but no thermodynamic data to get their P-T windows
Initiated Catalyst Screening for Mg$_2$Si Hydrogenation

- Synthesized Nano-Mg$_2$Si
- Synthesized and screened more than 20 catalysts
- No catalyst with observable activity was identified at 105°C under 60 atm H$_2$.
- Large amount of catalyst candidates remain unexplored

(a) RBS composition analysis

(b) XRD structure analysis
Future Work (FY06-07)

• Continue catalyst screening for MgH₂ + Si System
  – Optimize metal hydrides and catalysts preparation methods
  – Prepare and screen more catalysts for Mg₂Si hydrogenation
  – Start catalyst screening for MgH₂ + Si dehydrogenation
  – Milestones
    *Identify catalysts which lower the temperature for observable release to below 120°C to meet DOE’s P-T window requirements (June 2006)*
    *Identify catalysts which enable Mg₂Si hydrogenation (June 2006)*

• Catalyst screening for Li-Mg-N-H System
  – Collaborate with Sandia National Lab on metal hydride preparation and detailed catalyst characterization
  – Milestone
    *Identify catalysts which improve the hydrogen release rate to meet DOE 2010 targets and keep ammonia release below 1ppm at temperatures below 120°C (Sep. 2006)*
Future Work (FY06-07)

• Catalyst screening for LiBH$_4$ + MgH$_2$ System
  – Collaborate with HRL labs on metal hydride preparation and detailed catalyst characterization
  – Milestone
    *Identify catalysts which lower the temperature for observable hydrogen release to below 230°C (Sep. 2006)*

• Catalyst screening for other metal hydride candidates
  – Candidates include complex anionic materials, such as Ca and Mg borohydrides, and complex anionic alanates
Objective: Identify catalysts which improve the kinetics and selectivity for desired metal hydride systems to enable an on-board hydrogen storage system which meets DOE 2010 targets

Approaches: Combinatorial nano-catalyst synthesis and high throughput screening to speed up catalyst discovery

Technical Accomplishments and Progress:
(1) Design, setup and validated combinatorial nano-catalyst synthesis and high throughput catalyst screening processes
(2) Identified more than 15 systems as potential hydrogen storage candidates by thermodynamic calculation using HSC Chemistry®
(3) Initiated catalyst screening for Mg$_2$Si hydrogenation and no effective catalysts were identified so far

Proposed Future Research: Optimize synthesis and screening methods; Continue high throughput screening of catalysts for MgH$_2$ + Si, Li-Mg-N-H, LiBH$_4$ + MgH$_2$ and other potential candidates
Critical Assumptions and Issues

• Catalyst Synthesis
  – Obtaining alloy catalysts requires high temperature treatment; but metal hydride systems may decompose at such temperature
  – Screening may start with catalysts for hydrogenation instead of dehydrogenation; but the reversibility of some hydride systems may not be achieved

• High Throughput Screening
  – For metal hydrides with slow kinetics, elevated P&T are necessary for effective screening; but in-situ screening techniques can not be operated at such conditions
  – Use high P&T cell to run dehydrogenation and rehydrogenation without in-situ screening; and use ex-situ method to characterize the results