High Throughput Combinatorial Chemistry Development of Complex Hydrides

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Project ID:**STP7**

This presentation does not contain any proprietary or confidential information

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Overview

Timeline

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

Budget

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

Barriers

- Slow kinetics
- Low reversibility
- Release of undesired compounds

Partners

- HRL labs – MgH_2 + Si, $LiBH_4$ + MgH_2
- Sandia National Labs- Li-Mg-N-H
- Other partners for future collaborations

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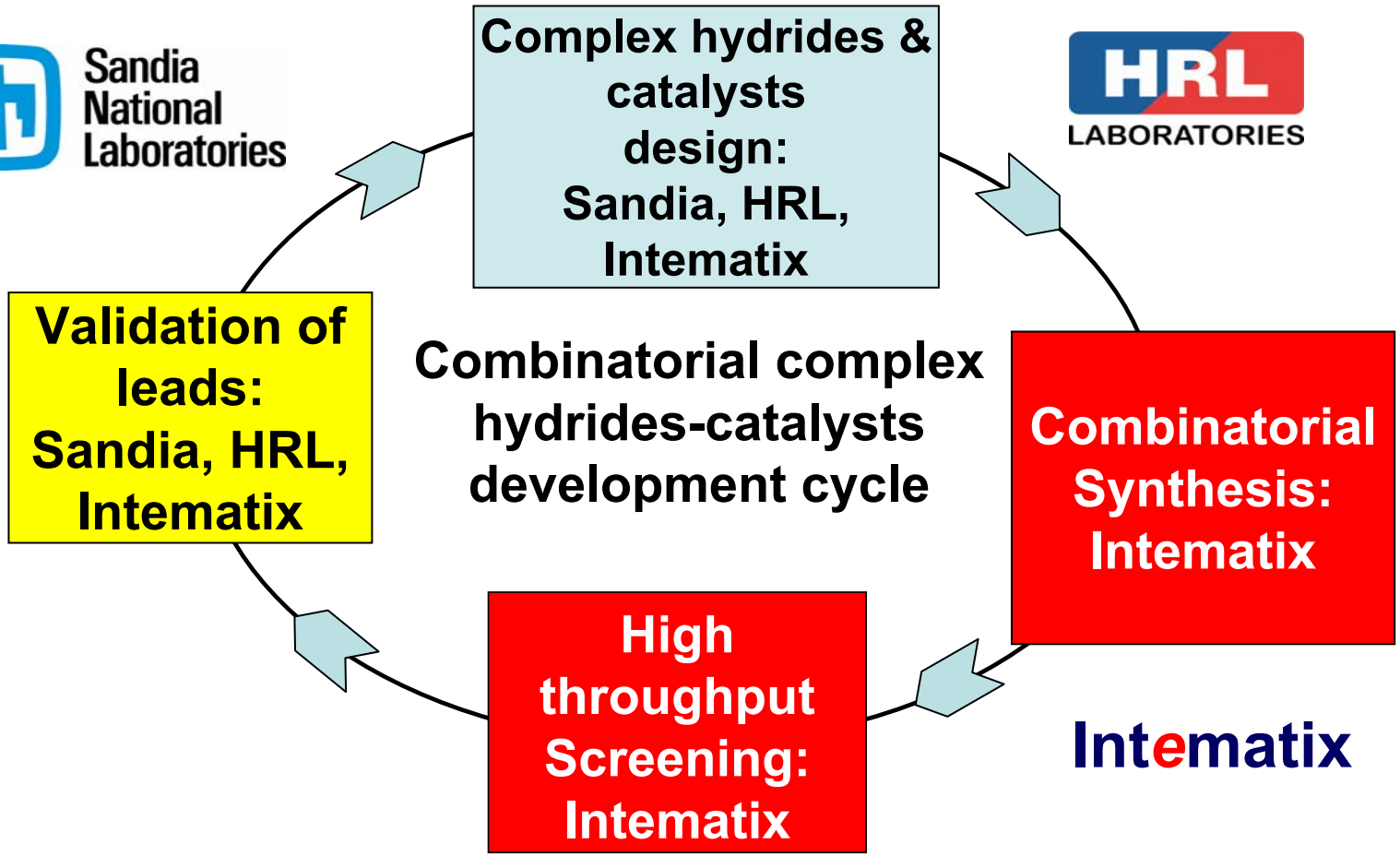
Objectives

- 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 H_2/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 MgH_2+Si system dehydrogenation and rehydrogenation
  - Screen catalysts for Li-Mg-N-H system dehydrogenation and rehydrogenation
  - Screen catalysts for $LiBH_4$+MgH_2 system dehydrogenation and rehydrogenation

Approach



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Approach

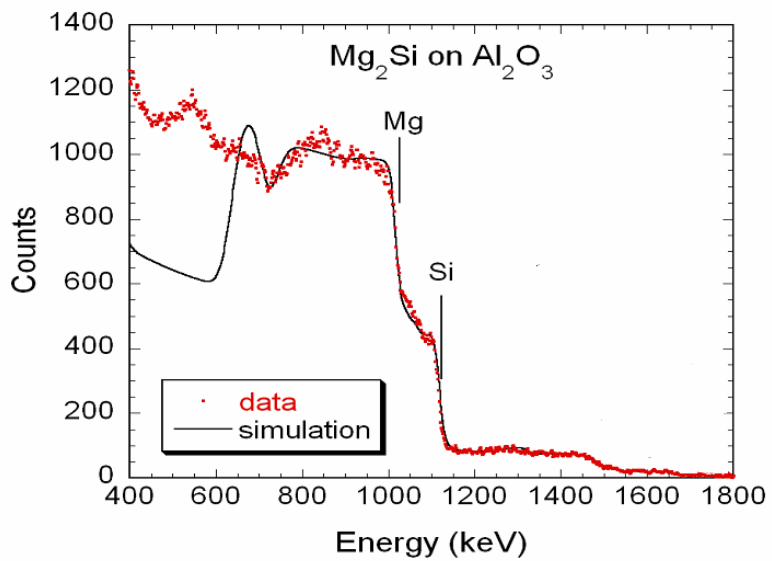
- Metal hydrides preparation
  - Study the chemical properties of metal hydride candidates
  - Design metal hydride synthesis process
- Combinatorial catalysts preparation
  - Design catalyst compositions
  - Design combinatorial nano-catalyst synthesis process
- High throughput screening of catalysts
  - 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

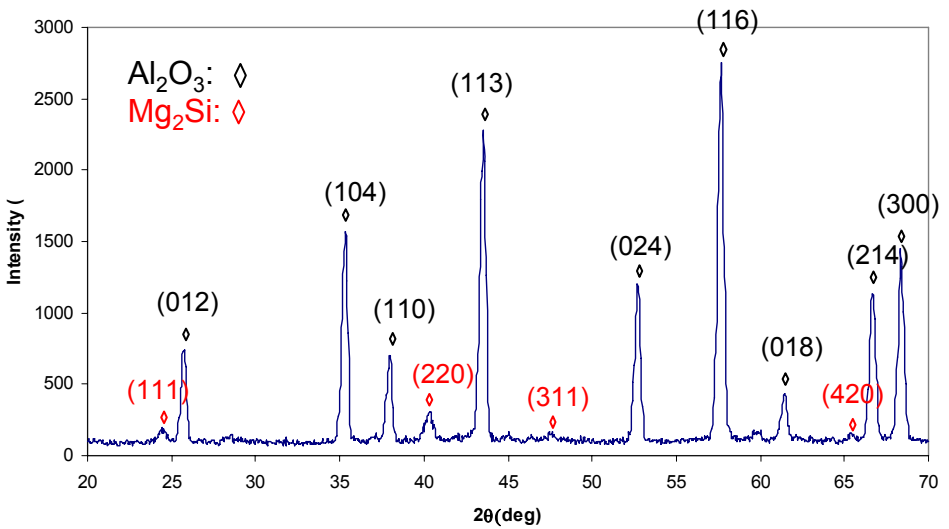
- Database search/calculations of ca. 200 candidate reactions using HSC Chemistry®
- Identified more than 15 reaction systems with > 6 wt% H_2 and P-T windows close to DOE targets
- Identified many potential reaction systems with high H_2 wt% but no thermodynamic data to get their P-T windows

Initiated Catalyst Screening for Mg_2Si Hydrogenation

- Synthesized Nano-Mg_2Si
- 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

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Future Work (FY06-07)

- Continue catalyst screening for MgH_2 + Si System
  - Optimize metal hydrides and catalysts preparation methods
  - Prepare and screen more catalysts for Mg_2Si hydrogenation
  - Start catalyst screening for MgH_2 + Si dehydrogenation
  - Milestones

    Identify catalysts which lower the temperature for observable release to below120°C to meet DOE's P-T window requirements (June 2006)

    Identify catalysts which enable Mg_2Si 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)

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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

Project Summary

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_2Si 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

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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