



**Hydrogen Storage Engineering**  
CENTER OF EXCELLENCE

# Chemical Hydride Rate Modeling, Validation, and System Demonstration

## LANL Engineering Team

***T.A. Semelsberger (P.I.) , Rod Borup, Eric Brosha, Jose Tafoya,  
Gerie Purdy, Mike Inbody, and Rangachary Mukundan***

***DOE Hydrogen Program Annual Merit Review,  
EERE: Hydrogen, Fuel Cells and Infrastructure Technologies Program***

***Washington, DC***

***May 18-22, 2009***

***Program Manager: Monterey Gardener***



**U.S. Department of Energy**

**Energy Efficiency and Renewable Energy**

Bringing you a prosperous future where energy is clean, abundant, reliable, and affordable



*This presentation does not contain any proprietary, confidential, or otherwise restricted information*

UNCLASSIFIED

**Project ID: stp\_09\_semelsberger**

# Introduction and Project Approach

---

Los Alamos National Laboratory's Chemical Hydride Rate Modeling, Validation, and System Demonstration Project is a newly funded DOE project under the Hydrogen Storage Engineering Center of Excellence led by SRNL. The scope of work for the Hydrogen Storage Engineering Center of Excellence are:

- Systems engineering for hydrogen storage systems for vehicular applications
- Energy management. Understand impact on subsystems of required heat and/or mass transport
- Novel component & reactor designs. Stress conformable designs that are compact and light-weight
- Concept evaluation & sub-scale prototype testing

In support of the goals and objectives of the Hydrogen Storage Engineering Center Excellence (HSECoE) , Los Alamos National Laboratory will contribute to modeling, designing, fabricating, and testing a prototype hydrogen release reactor for a hydrogen storage system based on chemical hydrides. Through these efforts, we plan to solve critical issues for implementation of chemical hydrides in a hydrogen storage system and develop two key enabling technologies for other hydrogen storage system types.

Los Alamos National Laboratory work scope includes:

- Develop Fuel Gauge Sensors for Hydrogen Storage Media
- Develop Models of the Aging Characteristics of Hydrogen Storage Materials
- Develop Rate Expressions of Hydrogen Release for Chemical Hydrides
- Develop Novel Reactor Designs for Start-up and Transient Operation for Chemical Hydrides
- Identify Hydrogen Impurities and Develop Novel Impurity Mitigation Strategies
- Design, Build, and Demonstrate a Subscale Prototype Reactor Using Liquid or Slurry Phase Chemical Hydrides

# LANL Project Overview

## Timeline

- Project Start Date: Feb FY09
- Project End Date: FY14
- Percent Complete: 5%

## Budget

- Total Project Funding: 4,651K
- Project End Date: FY14
- Funding:
  - 2009: \$578K
  - 2010: \$712K

## Barriers

### • Barriers Addressed

- *Efficiency*
- *Gravimetric Capacity*
- *Volumetric Capacity*
- *Durability/Operability*
- *H<sub>2</sub> Discharging Rates*
  - *Start time to full flow*
  - *Transient Response*
- *H<sub>2</sub> Purity*
- *Environmental, Health & Safety*

## Project Timeline

Phase 1								Phase 2						Phase 3					
2009				2010				2011				2012		2012		2013			
Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4

# HSECoE Partners

---



# LANL Project Objectives, Project Milestones & Project Go/No-Go Decision Points

Objectives and Tasks	Phase 1								Phase 2								Phase 3							
	FY09				FY10				FY11				FY12				FY13							
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4				
<b>Objective 1: To Act as the Chemical Hydrogen Storage Center of Excellence (CHSCoE) Liaison</b>																								
TASK 1.1: Identify and compile engineering modeling data for chemical hydrides							D4				D13				D18									
TASK 1.2: Provide testing protocols to CHSCoE							D6																	
TASK 1.3: Identify media risks and mitigation strategies							D7								D19									
<b>Objective 2: Develop Fuel Gauge Sensors for Hydrogen Storage Media</b>																								
TASK 2.1: Identify first generation fuel gauge sensors				D1				G1																
TASK 2.2: Develop and demonstrate fuel gauge sensors									M2						D20									
<b>Objective 3: Mathematically Model the Aging Characteristics of Candidate Hydrogen Storage Media</b>																								
TASK 3.1: Develop models to predict shelf-lives									M3						D21									
TASK 3.2: Provide accelerated aging testing protocols for shelf-life modeling to the HSMCoE				D2			D8																	
<b>Objective 4: Develop Rate Models for Hydrogen Release on Candidate Chemical Hydrides</b>																								
TASK 4.1: Identify operating temperatures and hydrogen release rates				D3																				
TASK 4.2: Collect kinetics data from CHSCoE and develop catalytic reaction rate models							D5																	
TASK 4.3: Model reactors with release kinetics coupled with mass and heat transfer effects								M1				D14												
TASK 4.4: Provide feedback to CHSCoE with strategies on catalyst optimization and design							D9					D15												
<b>Objective 5: Develop Novel Strategies for Start-Up and Transient Operation with Candidate Chemical Hydrides</b>																								
TASK 5.1: Identify reaction coupling schemes that minimize reactor start-up times and maximizing energy efficiency								D10																
TASK 5.2: Examine transient effects on reactor turn-down											M5				D22									
<b>Objective 6: Identify Hydrogen Impurities and Develop Novel Impurity Mitigation Strategies</b>																								
TASK 6.1: Identify impurities demonstrating fuel cell degradation								D11																
TASK 6.2: Determine adsorbate-adsorbent interactions												D16												
TASK 6.3: Quantify and model hydrogen impurities demonstrating fuel cell degradation								D12				D17												
TASK 6.4: Identify novel impurity separation strategies									M4			G2			D23									
DOE CENTER-WIDE GO/NO-GO												G3												
<b>Objective 7: Design, Build, and Demonstrate a Subscale Prototype Reactor that Releases Hydrogen using Chemical Hydrides</b>																								
TASK 7.1: Coordinate risk assessment and mitigation strategies for demonstration																D27								
TASK 7.2: Coordinate the integration of the relevant design concepts into the prototype design											M6				D24									
TASK 7.3: Coordinate the development of a logistics plan for testing and evaluating prototypes															G4									
TASK 7.4: Coordinate the development of decommissioning plans for subscale prototypes																D25								
TASK 7.5: Scale and design an optimized chemical hydride prototype																D26								
TASK 7.6: Fabricate subscale system components for chemical hydride prototype													M7						D28					
TASK 7.7: Build subscale chemical hydride test bed station																M8								
TASK 7.8: Assemble and evaluate subscale chemical hydride prototype																M9			D29					
TASK 7.9: Coordinate the decommissioning of all subscale prototypes																M10				D30				
																				D31				

# LANL Project Deliverables

Phase	Deliverable	Description	Delivery to	Date
Phase 1	D1	First generation fuel gauge sensor	DOE	Q4 FY09
	D2	Testing protocols for shelf-life data acquisition	CHSCoE	Q4 FY09
	D3	Identify the operating conditions for rate data collection	CHSCoE	Q4 FY09
	D4	Identify & compile engineering data for chemical hydrides	DOE & ECoE	Q2 FY10
	D5	Collate rate data collected by the CHSCoE and develop rate model	ECoE	Q2 FY10
	D6	Provide testing protocols to CHSCoE	CHSCoE	Q3 FY10
	D7	Identify & compile chemical hydride media risks and mitigation strategies	DOE & ECoE	Q4 FY10
	D8	Update testing protocols for shelf-life data acquisition (as needed)	CHSCoE	Q4 FY10
	D9	Provide feedback to CHSCoE on potential catalyst optimization strategies	CHSCoE	Q4 FY10
	D10	Reaction coupling schemes addressing start-up and transient operation	CHSCoE, ECoE, & DOE	Q4 FY10
	D11	Identify fuel cell impurities	DOE, HSMCoE, & ECoE	Q4 FY10
	D12	Quantify minimum fuel-cell impurity level for safe operation	DOE & ECoE	Q4 FY10
Phase 2	D13	Update engineering data for chemical hydrides (as needed)	DOE & ECoE	Q3 FY11
	D14	Rate model for chemical hydride hydrogen release	DOE & ECoE	Q4 FY11
	D15	Provide update to CHSCoE on potential catalyst optimization strategies	CHSCoE	Q4 FY11
	D16	Determine fuel cell degradation via impurities	DOE & ECoE	Q4 FY11
	D17	Update on minimum fuel-cell impurity level for safe operation	DOE & ECoE	Q4 FY11
	D18	Update engineering data for chemical hydrides (as needed)	DOE & ECoE	Q2 FY12
	D19	Update chemical hydride media risks and mitigation strategies	DOE & ECoE	Q2 FY12
	D20	Working fuel gauge sensor capable of monitoring H2 levels within +/- 5%	DOE & ECoE	Q2 FY12
	D21	Shelf-life models for candidate hydrogen storage media	DOE & ECoE	Q2 FY12
	D22	Report on transient operation of novel reaction coupling schemes	DOE & ECoE	Q2 FY12
	D23	Working Impurity mitigation device with low cost, low volume & low mass	DOE & ECoE	Q2 FY12
	D24	Final prototype designs for all media types	DOE & ECoE	Q2 FY12
Phase 3	D25	Logistics plan for testing and evaluating subscale prototypes	DOE & ECoE	Q3 FY12
	D26	Decommissioning plans for SRNL, JPL, & LANL	DOE & ECoE	Q3 FY12
	D27	Report on all known risks and mitigation strategies for prototype demonstrations	DOE & ECoE	Q4 FY12
	D28	Final scaled design of all prototypes	DOE & ECoE	Q1 FY13
	D29	Test bed proper for demonstrating subscale prototype	DOE & ECoE	Q2 FY13
	D30	Final assembly and evaluation of subscale prototypes	DOE & ECoE	Q4 FY13
	D31	Prototype decommissioning	DOE & ECoE	Q4 FY13

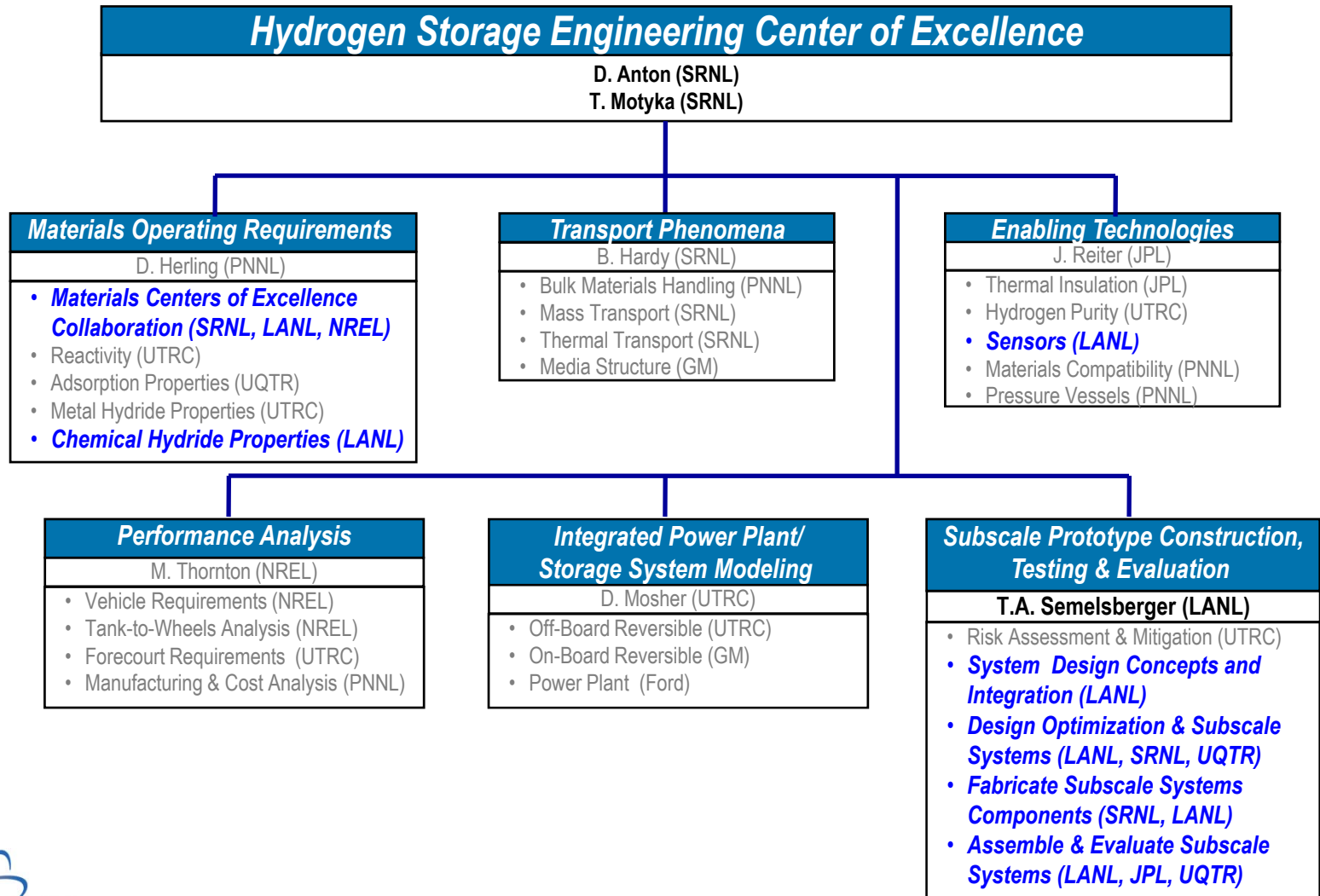
# LANL Project Milestones and Go/No-Go Decisions

Phase	Milestone	Description	Dependencies	Date
Phase 1	M1	Reactor model with release kinetics coupled with heat and mass	TASKS 4.1 and 4.2	Q4 FY10
Phase 2	M2	Fuel gauge sensor development and demonstration	TASK 2.1	Q1 FY11
	M3	Shelf-life model development	TASK 3.2	Q1 FY11
	M4	Impurity mitigation strategy development	TASKS 6.1 and 6.3	Q1 FY11
	M5	Examination of transient effects on reactor turn-down	TASK 5.1	Q3 FY11
	M6	Integration of most promising design concepts in subscale prototypes	ECoE TASKS	Q3 FY11
	M7	Scale and design chemical hydride prototype system proper	TASK 7.2	Q1 FY12
Phase 3	M8	Fabricate subscale system components	TASK 7.5	Q3 FY12
	M9	Build subscale chemical hydrided test bed station	TASK 7.6	Q4 FY12
	M10	Assemble and evaluate subscale chemical hydride prototype	TASK 7.7	Q1 FY13

Phase	Go/No-Go	Description	Criteria*	Date
Phase 1	G1	Go/No-Go Decision on fuel gauge sensor	+/- 5% of H <sub>2</sub> Stored	Q4 FY10
Phase 2	G2	Go/No-Go Decision on viable impurity mitigation/separation strategies	mass, volume, cost	Q4 FY11
	G3	DOE Center-Wide Go/No-Go for Continuing to Phase 3	volume, cost, mass	Q4 FY11
	G4	Go/No-Go decisions on integrated design concepts for each prototype	efficiency, mass, volume, cost	Q2 FY12

*\* all Go/No-Go decisions will be based on the most current DOE Technical Targets; the components or designs that most favorably compare to the DOE Technical Targets will be chosen*

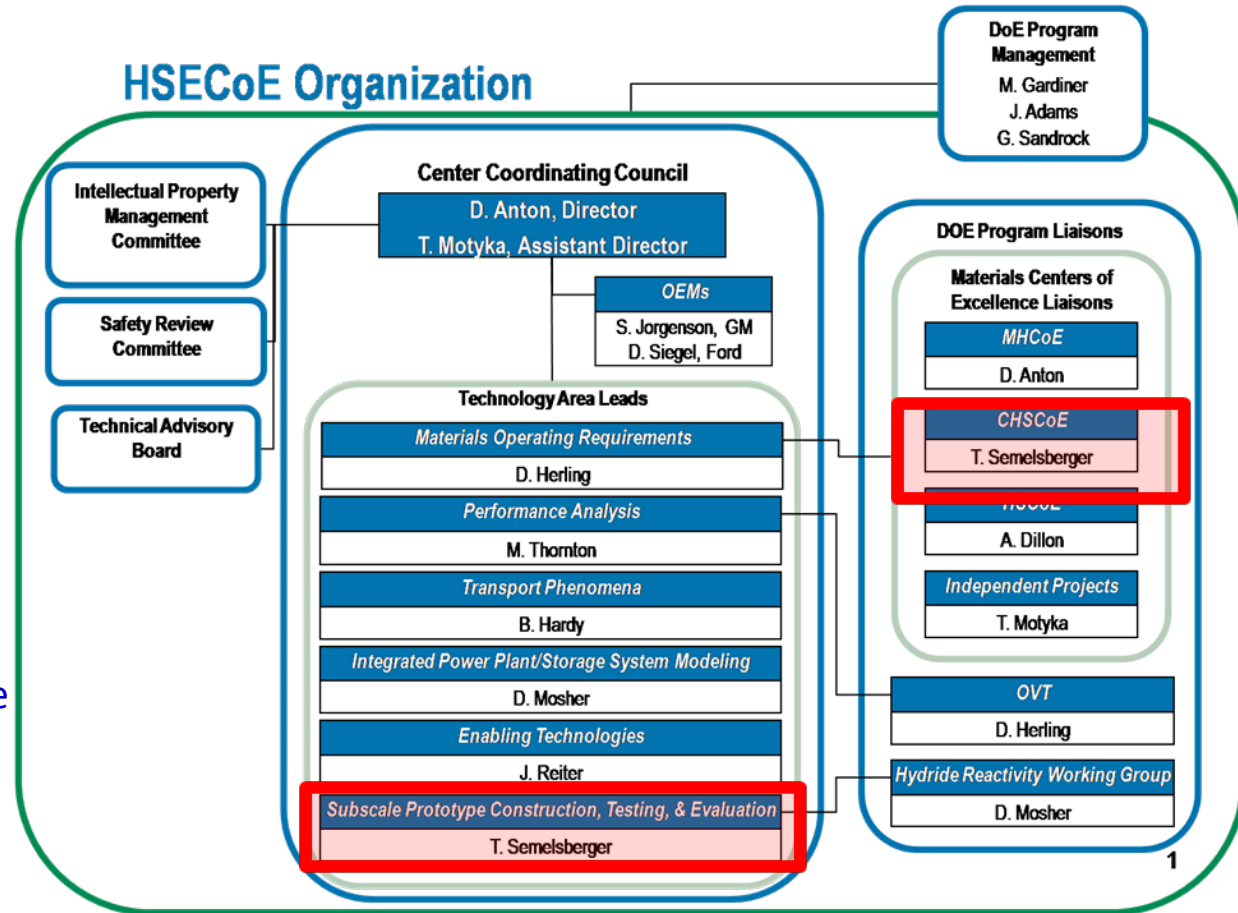
# LANL Management Roles in the HSECoE



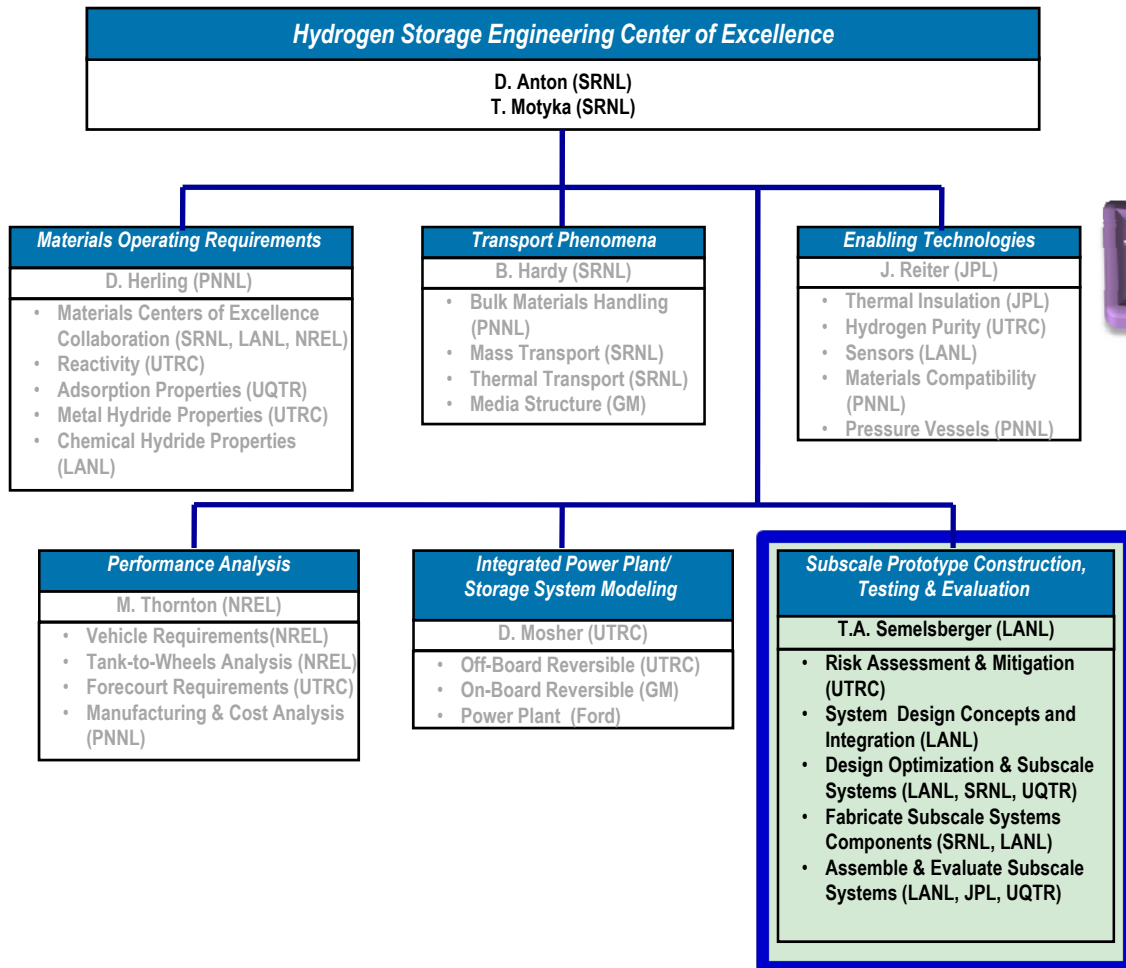


# LANL Management Tasks in Support of HSECoE

- Technology Area Leader (TAL) for the Subscale Prototype Construction, Testing, & Evaluation Technology Area
- Technology Area Team Lead:
  - Chemical Hydride Properties
  - Sensors
  - System Design Concepts and Integration
  - Design and Optimize Subscale Prototype
  - Fabricate Subscale System Component
  - Assemble and Demonstrate Subscale Prototypes
- DOE Program Liaison to the Chemical Hydrogen Storage Center of Excellence (CHSCoE)



# HSECoE Technology Areas and Technology Area Teams



# Technology Area Lead (TAL): Subscale Prototype Construction, Testing and Evaluation

---

## General Roles of TAL

- Provide rapid dissemination of information
- Maintain project continuity and progress
- Coordinate and Assist Technology Area Teams
- Interface with other TALs and Center Director

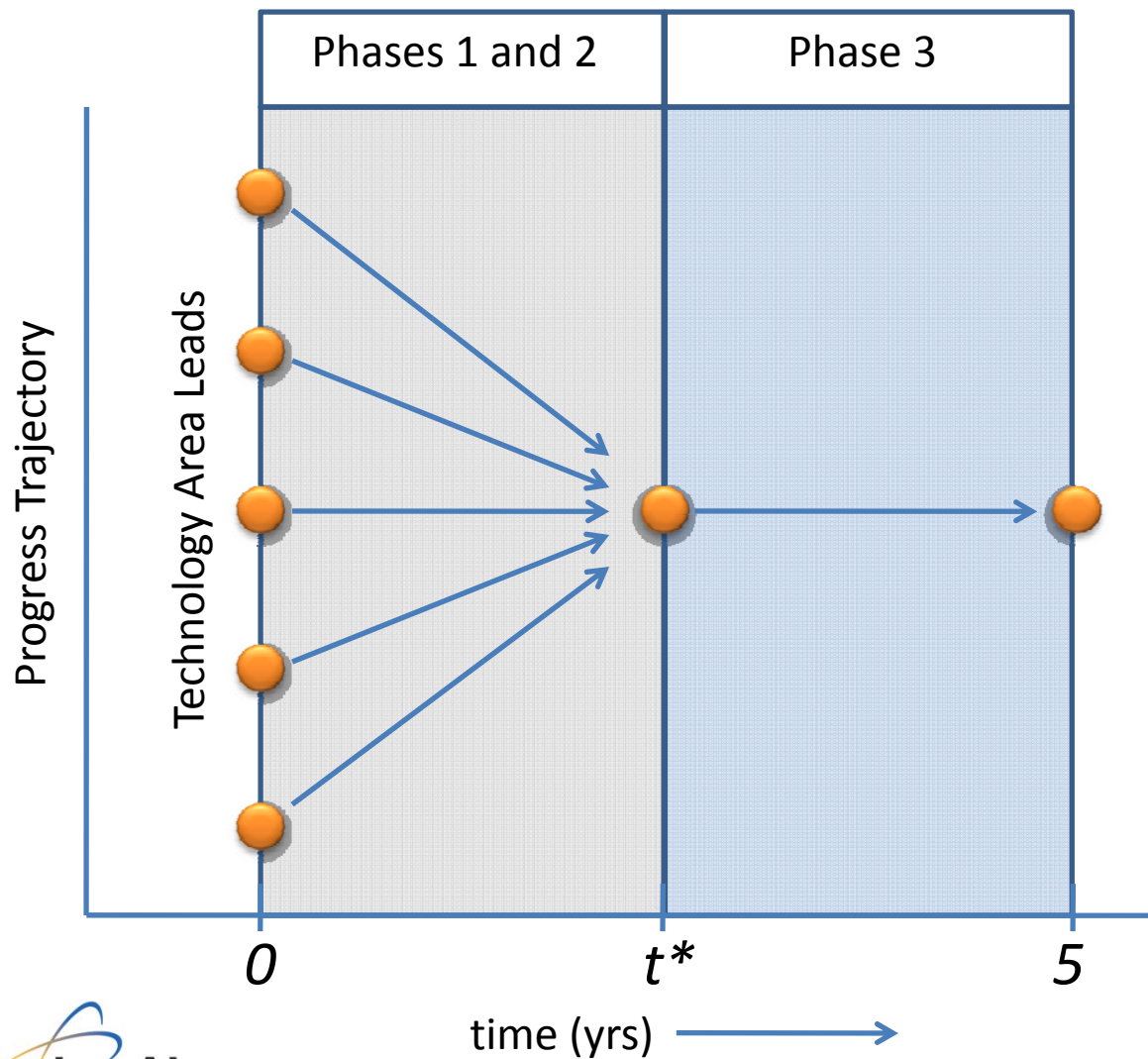
## Specific Responsibilities of TAL

- Ensure health and safety protocols are in place at testing facilities prior to prototype demonstration
- Ensure decommissioning plans are documented and in place
- Coordinate prototype construction, testing, and evaluation
- Compile and disseminate systems risks and mitigation strategies
- DOE reporting

# Roles and Responsibilities of Technology Area Teams in Subscale Prototype Construction and Evaluation

	Technology Area Teams	Collaborators	Roles and Responsibilities
Technology Area: Subscale Prototype Construction, Testing, and Evaluation (TAL: LANL)	Risk Assessment & Mitigation	UTRC	Lead risk assessments for prototype fabrication, testing, and decommissioning
		All Partners	
	System Design Concepts and Integration	LANL All Partners	LANL will coordinate the integration of relevant component design concepts into the prototype demonstration units
	Prototype Assembly and Evaluation	LANL	Lead the assembly, test stand construction, evaluation, and decommissioning of liquid or slurry phase chemical hydrides
		JPL	Lead metal hydride subscale prototype final assembly, test stand construction and evaluation
		UQTR	Lead the assembly, testing, and decommissioning of sorption materials
	Prototype Fabrication	LANL	Lead the fabrication efforts of the subscale prototype for chemical hydride prototype evaluation
		UTRC	Fabricate on-board separation components for all prototype demonstrations
		SRNL	Lead fabrication efforts of subscale metal hydrides and sorption material prototypes and components
		JPL	Lead hardware fabrication and validation testing for metal hydrides and sorption materials heat exchange components
		PNNL	Lead the fabrication efforts of conformal tank design
		Lincoln	Fabricate composite vessels for metal hydrides and sorption materials
		OSU	Fabricate microchannel heat exchangers for both metal hydrides and sorption materials
	Prototype Design and Optimization	LANL	Scale and design novel liquid or slurry phase chemical hydride reactor
		UTRC	Support heat exchanger design modeling led by SRNL for metal hydrides and sorption materials
		SRNL	Lead design of subscale metal hydrides and sorption material prototypes and components
		PNNL	Design and optimize subscale chemical hydride prototype microchannel heat exchanger and lead conformal tank design with Lincoln and UTRC
		JPL	Lead thermal insulation design efforts
		Lincoln	Design, build and test composite vessels for various conformal architectures
		OSU	Model, design, and evaluate microchannel heat exchangers for metal hydrides and sorption materials

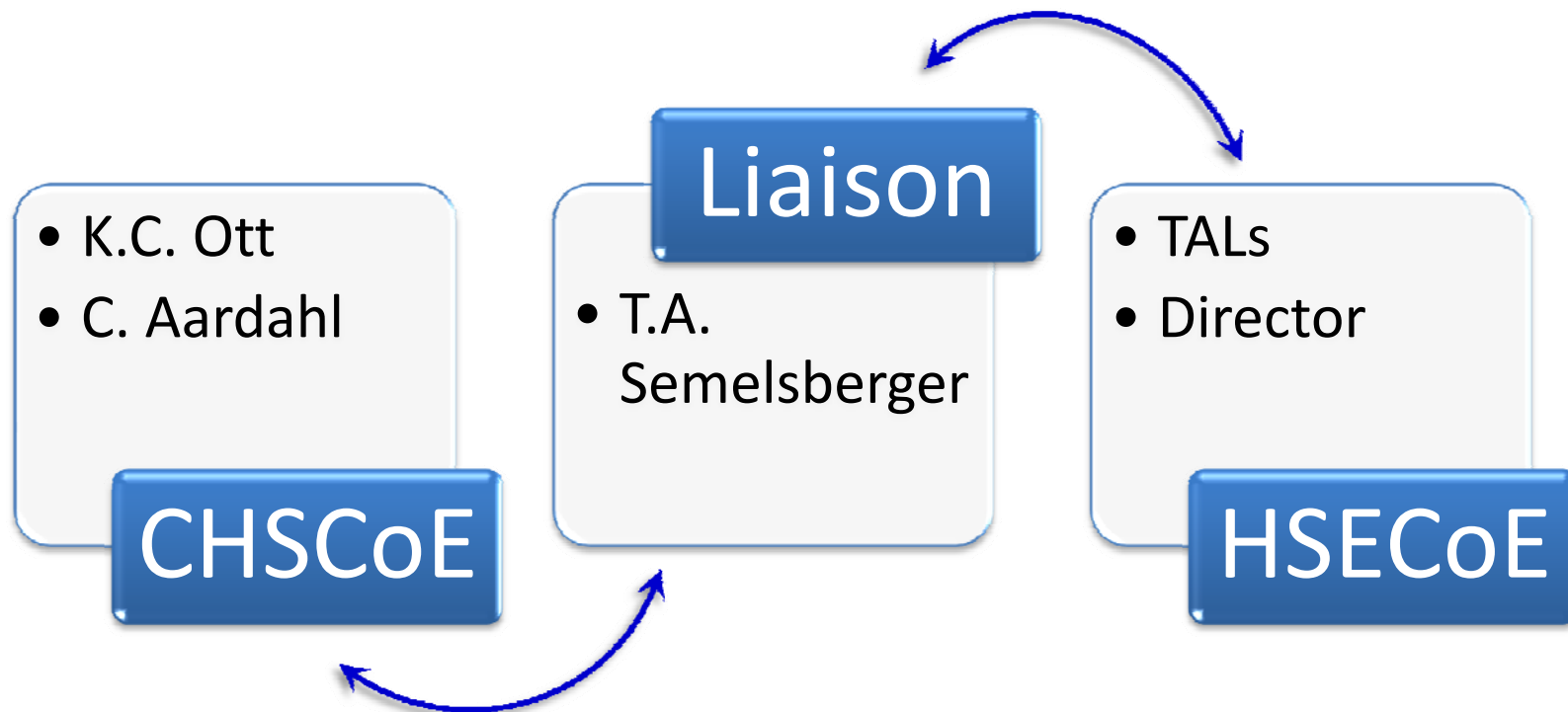
# Technology Area Leads and Liaisons are Critical to HSECoE Success



## Critical Issues for Success

- Communication among Technology Area Leads for course corrections
- Center Meetings
- Technology Area Team Meetings
  - ✓ Monthly telecons
- Communication between DOE Program Liaisons
- Down selection

# DOE Program Liaison to Chemical Hydrogen Storage Center of Excellence(CHSCoE)



Role of Liaison: Interface with CHSCoE

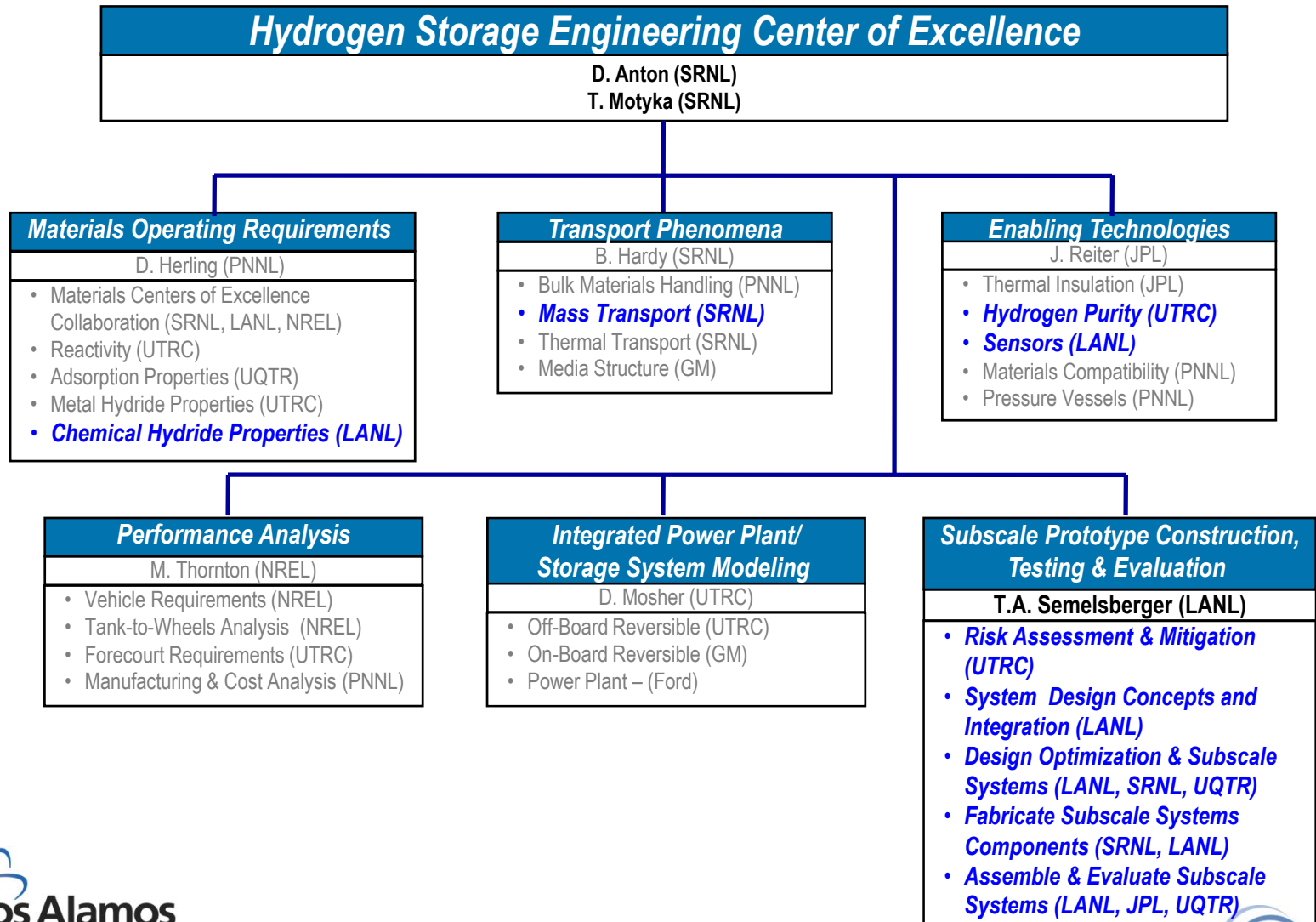
# DOE Program Liaison to Chemical Hydrogen Storage Center of Excellence(CHSCoE)

---

## Responsibilities of CHSCoE Liaison

- Identify and compile engineering data for chemical hydrogen storage media
- Identify Information/knowledge/technology gaps
- Collaborate with CHSCoE on reactor testing chemical hydrides and catalysts
- Collaborate with D. Herling (TAL), D. Mosher and CHSCoE to identify media risks and mitigation strategies
- DOE Reporting

# LANL Primary Technical Contribution Areas





# LANL Engineering Objectives in Support of HSECoE

---

## LANL Engineering Objectives

**Objective 2: Develop Fuel Gauge Sensors for Hydrogen Storage Media**

**Objective 3: Develop Models of the Aging Characteristics of Hydrogen Storage Materials**

**Objective 4: Develop Rate Expressions of Hydrogen Release for Chemical Hydrides**

**Objective 5: Develop Novel Reactor Designs for Start-up and Transient Operation for Chemical Hydrides**

**Objective 6: Identify Hydrogen Impurities and Develop Novel Impurity Mitigation Strategies**

**Objective 7: Design, Build, and Demonstrate a Subscale Prototype Reactor Using Liquid or Slurry Phase Chemical Hydrides**

# Objective 2: Fuel Gauge Sensor Development

---

## ✓ Relevance:

- DOE Targets Addressed: N/A
- All commercialized vehicles necessitate a fuel gauge sensor

## ✓ Expected Outcomes:

- Fuel gauge sensor for solid- and slurry-phase hydrogen storage media

## ✓ Tasks:

- 2.1 Identify first generation fuel gauge sensors
- 2.2 Demonstrate fuel gauge sensor technology on candidate hydrogen storage media

✓ LANL Personnel: E. L. Brosha and R. Mukundan

# Objective 2: Fuel Gauge Sensor Development

Objectives and Tasks	Phase 1				Phase 2				Phase 3							
	FY09		FY10		FY11		FY12		FY13							
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
<b>Objective 2: Develop Fuel Gauge Sensors for Hydrogen Storage Media</b>																
TASK 2.1: Identify first generation fuel gauge sensors	.	.	.	D1	.	.	.	G1	.	.	.	.	.	.	.	.
TASK 2.2: Develop and demonstrate fuel gauge sensors	.	.	.	.	.	.	.	.	M2	.	.	.	.	D20	.	.

❖ Deliverables	Phase	Deliverable	Description	Delivery to	Date
	Phase 1	D1	First generation fuel gauge sensor	DOE	Q4 FY09
	Phase 2	D20	Working fuel gauge sensor capable of monitoring H2 levels within +/- 5%	DOE & ECoE	Q2 FY12

❖ Go/No-Go	Phase	Go/No-Go	Description	Criteria*	Date
	Phase 1	G1	Go/No-Go Decision on fuel gauge sensor	+/- 5% of H <sub>2</sub> Stored	Q4 FY10
	<i>* all Go/No-Go decisions will be based on the most current DOE Technical Targets; the components or designs that most favorably compare to the DOE Technical Targets will be chosen</i>				

❖ Milestone	Phase	Milestone	Description	Dependencies	Date
	Phase 2	M2	Fuel gauge sensor development and demonstration	TASK 2.1	Q1 FY11

# Objective 3: Shelf-life Modeling

---

## ✓ Relevance:

- DOE Targets Addressed:
  - Cost
  - Durability and Operability
  - Environmental, Health and Safety

## ✓ Expected Outcomes:

- Key variables (i.e., time, temperature, pressure, humidity, and geographic location) required for the safe and effective storage of hydrogen storage media both on-board and at the production plant.
- Updated cost models regarding production plant size, production plant storage capacity, and frequency of regeneration

## ✓ Tasks:

- 3.1 Develop models to predict shelf lives of hydrogen storage media
- 3.2 Provide accelerated aging protocols for shelf life modeling to the HSMCoE

- ✓ LANL Personnel: T.A. Semelsberger and G. Purdy

# Objective 3: Shelf-life Modeling

	Phase 1				Phase 2				Phase 3							
	FY09		FY10		FY11		FY12		FY13							
Objectives and Tasks	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
<b>Objective 3: Mathematically Model the Aging Characteristics of Candidate Hydrogen Storage Media</b>																
TASK 3.1: Develop models to predict shelf-lives									M3					D21		
TASK 3.2: Provide accelerated aging testing protocols for shelf-life modeling to the HSMCoE			D2				D8									

❖ Deliverables	Phase	Deliverable	Description	Delivery to	Date	
	Phase 1	D2	Testing protocols for shelf-life data acquisition		CHSCoE	Q4 FY09
		D8	Update testing protocols for shelf-life data acquisition (as needed)		CHSCoE	Q4 FY10
	Phase 2	D21	Shelf-life models for candidate hydrogen storage media		DOE & ECoE	Q2 FY12

❖ Milestone	Phase	Milestone	Description	Dependencies	Date
	Phase 2	M3	Shelf-life model development		TASK 3.2

# Objective 4: Develop Reaction Rate Models for H<sub>2</sub> Release on Candidate Chemical Hydrides

## ✓ Relevance:

- DOE Targets Addressed:
  - Charging/Discharging Rates
  - Efficiency
  - Cost
  - Hydrogen Purity
  - Gravimetric and Volumetric Capacity

$$V_{reactor} = F_{A_o} \int_0^X \frac{dX}{-r_A}$$

## ✓ Expected Outcomes:

- Rate models for reactor design and operation

## ✓ Tasks:

- 4.1 Identify operating conditions and H<sub>2</sub> release rates for the state-of-the-art catalysts
- 4.2 Collate kinetics data from CHSCoE and develop rate models
- 4.3 Model reactors with coupled heat, mass, momentum, and kinetics
- 4.4 Provide feedback to CHSCoE with strategies on catalyst optimization and design

## ✓ Personnel:

T. A. Semelsberger and CHSCoE

## ✓ Deliverable:

- Rate expression for reactor design (Q2 FY10)

# Objective 4: Develop Reaction Rate Models for H<sub>2</sub> Release on Candidate Chemical Hydrides

Objectives and Tasks	Phase 1								Phase 2				Phase 3							
	FY09				FY10				FY11				FY12				FY13			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
<b>Objective 4: Develop Rate Models for Hydrogen Release on Candidate Chemical Hydrides</b>																				
TASK 4.1: Identify operating temperatures and hydrogen release rates for the state-of-the-art catalysts				D3																
TASK 4.2: Collect kinetics data from CHSCoE and develop catalytic reaction rate models								D5												
TASK 4.3: Model reactors with release kinetics coupled with mass and heat transfer effects												M1				D14				
TASK 4.4: Provide feedback to CHSCoE with strategies on catalyst optimization and design								D9								D15				

❖ Deliverables	Phase	Deliverable	Description	Delivery to	Date
	Phase 1	D3	Identify the operating conditions for rate data collection	CHSCoE	Q4 FY09
		D5	Collate rate data collected by the CHSCoE and develop rate model	ECoE	Q2 FY10
		D9	Provide feedback to CHSCoE on potential catalyst optimization strategies	CHSCoE	Q4 FY10
	Phase 2	D14	Rate model for chemical hydride hydrogen release	DOE & ECoE	Q4 FY11
		D15	Provide update to CHSCoE on potential catalyst optimization strategies	CHSCoE	Q4 FY11

❖ Milestone	Phase	Milestone	Description	Dependencies	Date
	Phase 1	M1	Reactor model with release kinetics coupled with heat and mass	TASKS 4.1 and 4.2	Q4 FY10

# Objective 5: Novel Reactor Designs for Startup and Transient Operation

---

## ✓ Relevance:

- DOE Targets Addressed:
  - Charging/Discharging Rates
  - Efficiency
  - Cost
  - Hydrogen Purity
  - Gravimetric and Volumetric Capacity

## ✓ Expected Outcomes:

- Novel reactor designs addressing startup and transient operation

## ✓ Tasks:

- 5.1 Identify reaction coupling schemes that minimize reactor start-up times and maximize energy efficiency
- 5.2 Examine transient effects on reactor turn-down

## ✓ Personnel: T.A. Semelsberger and CHSCoE



# Objective 5: Novel Reactor Designs for Startup and Transient Operation

Objectives and Tasks	Phase 1								Phase 2								Phase 3							
	FY09				FY10				FY11				FY12				FY13							
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4				
<b>Objective 5: Develop Novel Strategies for Start-Up and Transient Operation with Candidate Chemical Hydrides</b>																								
TASK 5.1: Identify reaction coupling schemes that minimize reactor start-up times and maximizing energy efficiency								D10																
TASK 5.2: Examine transient effects on reactor turn-down											M5				D22									

## ❖ Deliverables

Phase	Deliverable	Description	Delivery to	Date
Phase 1	D10	Reaction coupling addressing start-up and transient operation	CHSCoE, ECoE, & DOE	Q4 FY10
Phase 2	D22	Report on transient operation of novel reaction coupling schemes	DOE & ECoE	Q2 FY12

## ❖ Milestone

Phase	Milestone	Description	Dependencies	Date
Phase 2	M5	Examination of transient effects on reactor turn-down	TASK 5.1	Q3 FY11

# Objective 6: Hydrogen Impurities and Mitigation

---

## ✓ Relevance:

### • DOE Targets Addressed:

- Cost
- Durability and Operability
- Environmental, Health and Safety
- Fuel Purity

## ✓ Expected Outcomes:

- Impurities demonstrating fuel cell degradation for all candidate storage materials
- Strategies for impurity mitigation/separation

## ✓ Tasks:

- 6.1 Identify impurities demonstrating fuel cell degradation
- 6.2 Determine adsorbate-adsorbent interactions
- 6.3 Quantify and model hydrogen impurities demonstrating fuel cell degradation
- 6.4 Identify novel impurity separation/mitigation strategies

## ✓ Personnel: R. Borup and CHSCoE

## ✓ Go/No-Go Decision Criterion:

- DOE Technical Target of 99.99% H<sub>2</sub> purity (Q4 FY11)

# Objective 6: Hydrogen Impurities and Mitigation

Objectives and Tasks	Phase 1								Phase 2				Phase 3							
	FY09				FY10				FY11				FY12				FY13			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
<b>Objective 6: Identify Hydrogen Impurities and Develop Novel Impurity Mitigation Strategies</b>																				
TASK 6.1: Identify impurities demonstrating fuel cell degradation								D11												
TASK 6.2: Determine adsorbate-adsorbent interactions												D16								
TASK 6.3: Quantify and model hydrogen impurities demonstrating fuel cell degradation								D12				D17								
TASK 6.4: Identify novel impurity separation strategies									M4			G2			D23					

❖ Deliverables	Phase	Deliverable	Description	Delivery to	Date
	Phase 1	D11	Identify fuel cell impurities	DOE, HSMCoE, & ECoE	Q4 FY10
		D12	Quantify minimum fuel-cell impurity level for safe operation	DOE & ECoE	Q4 FY10
	Phase 2	D16	Determine fuel cell degradation via impurities	DOE & ECoE	Q4 FY11
		D17	Update on minimum fuel-cell impurity level for safe operation	DOE & ECoE	Q4 FY11
		D23	Working Impurity mitigation device with low cost, low volume & low mass	DOE & ECoE	Q2 FY12

❖ Milestone	Phase	Milestone	Description	Dependencies	Date
	Phase 2	M4	Impurity mitigation strategy development	TASKS 6.1 and 6.3	Q1 FY11

❖ Go/No-Go	Phase	Go/No-Go	Description	Criteria	Date
	Phase 2	G2	Go/No-Go Decision on viable impurity mitigation/separation strategies	mass, volume, cost, purity	Q4 FY11

# Objective 7: Design, Build, & Demonstrate Subscale Chemical Hydride Prototype

## ✓ Relevance:

The crowning deliverable of the DOE HSECoE is the demonstration of a subscale on-board hydrogen storage prototype for each of the material-based technologies addressing the DOE technical targets.

## ✓ Expected Outcomes:

- In-depth knowledge of the underlying subtleties of engineering an automotive hydrogen-storage based vehicle
- Guidance for DOE on future research directions

## ✓ Tasks:

- 7.1 Coordinate risk assessment and mitigation strategies for demonstration
- 7.2 Coordinate the integration of the most relevant design concepts in subscale prototypes
- 7.3 Coordinate the logistics plan for testing and evaluating subscale prototypes
- 7.4 Coordinate the development of the decommissioning plans of prototype demonstrations
- 7.5 Coordinate scaling and designing the chemical hydride prototype reactor
- 7.6 Coordinate the fabrication of subscale components for chemical hydride prototype
- 7.7 Build subscale chemical hydride test bed proper
- 7.8 Assemble and evaluate subscale chemical hydride prototype unit
- 7.9 Coordinate the decommissioning of all subscale prototypes

## ✓ Go/No-Go Decision Criterion:

- DOE Go/No-Go Decision (Q4 FY12)

## ✓ Deliverable:

Demonstrated prototype (Q4 FY13)

✓ Personnel: T. A. Semelsberger, M. Inbody, J. Tafoya, E. Brosha, & G. Purdy

# Objective 7: Design, Build, & Demonstrate Subscale Chemical Hydride Prototype

Objectives and Tasks	Phase 1								Phase 2								Phase 3							
	FY09				FY10				FY11				FY12				FY13							
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4				
<b>Objective 7: Design, Build, and Demonstrate a Subscale Prototype Reactor that Releases Hydrogen using Chemical Hydrides</b>																								
TASK 7.1: Coordinate risk assessment and mitigation strategies for demonstration																				D27				
TASK 7.2: Coordinate the integration of the most relevant design concepts into the subscale prototype design										M6				D24						G4				
TASK 7.3: Coordinate the development of a logistics plan for testing and evaluating subscale prototypes																D25								
TASK 7.4: Coordinate the development of decommissioning plans for subscale prototypes																D26								
TASK 7.5: Scale and design an optimized chemical hydride prototype														M7						D28				
TASK 7.6: Fabricate subscale system components for chemical hydride prototype																		M8						
TASK 7.7: Build subscale chemical hydride test bed station																			M9	D29				
TASK 7.8: Assemble and evaluate subscale chemical hydride prototype																			M10	D30				
TASK 7.9: Coordinate the decommissioning of all subscale prototypes																				D31				

# Objective 7: Design, Build, & Demonstrate Subscale Chemical Hydride Prototype

## ❖ Deliverables

Phase	Deliverable	Description	Delivery to	Date
Phase 2	D23	Working Impurity mitigation device with low cost, low volume & low mass	DOE & ECoE	Q2 FY12
	D24	Final prototype designs for all media types	DOE & ECoE	Q2 FY12
Phase 3	D25	Logistics plan for testing and evaluating subscale prototypes	DOE & ECoE	Q3 FY12
	D26	Decommissioning plans for SRNL, JPL, & LANL	DOE & ECoE	Q3 FY12
	D27	Report on all known risks and mitigation strategies for prototype demonstrations	DOE & ECoE	Q4 FY12
	D28	Final scaled design of all prototypes	DOE & ECoE	Q1 FY13
	D29	Test bed proper for demonstrating subscale prototype	DOE & ECoE	Q2 FY13
	D30	Final assembly and evaluation of subscale prototypes	DOE & ECoE	Q4 FY13
	D31	Prototype decommissioning	DOE & ECoE	Q4 FY13

## ❖ Milestone

Phase	Milestone	Description	Dependencies	Date
Phase 2	M6	Integration of most promising design concepts in subscale prototypes	ECoE TASKS	Q3 FY11
	M7	Scale and design chemical hydride prototype system proper	TASK 7.2	Q1 FY12
Phase 3	M8	Fabricate subscale system components	TASK 7.5	Q3 FY12
	M9	Build subscale chemical hydride test bed station	TASK 7.6	Q4 FY12
	M10	Assemble and evaluate subscale chemical hydride prototype	TASK 7.7	Q1 FY13

## ❖ Go/No-Go

Phase	Go/No-Go	Description	Criteria	Date
Phase 2	G4	Go/No-Go decisions on integrated design concepts for each prototype	efficiency, mass, volume, cost	Q2 FY12

# FY 2009 Activities and Deliverables

## ❖ Activities

- Identify and compile engineering data for candidate chemical hydrides
- Develop testing protocols for reactor kinetics experiments
- Identify and disseminate hydrogen storage material safety concerns
- Explore fuel gauge sensor technologies
- Identify accelerated aging testing protocols
- Identify reactor operating conditions for state-of-the-art catalysts
- Identify potential reaction coupling schemes for startup and transient operation
- Develop protocols and test bed proper for hydrogen impurities task
- Acquire various metal hydrides and chemical hydrides for impurity testing and fuel gauge sensor development

## ❖ Deliverables

- Quarterly reports on progress
- Disseminate kinetics testing protocols to HSCoE (Q4 2009)
- Develop and disseminate accelerated aging protocols to HSCoE (Q4 2009)
- First generation fuel gauge sensor (Q4 2009)

# Acknowledgements

---



**U.S. Department of Energy**  
**Energy Efficiency  
and Renewable Energy**

Bringing you a prosperous future where energy  
is clean, abundant, reliable, and affordable

Hydrogen, Fuel Cells & Infrastructure Technologies Program:  
Hydrogen Storage  
Manager: Monterey Gardiner