Discovery of Novel Complex Metal Hydrides for Hydrogen Storage through Molecular Modeling and Combinatorial Methods

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Project Objectives

- **Discovery of a complex metal hydride through Molecular Modeling and Combinatorial Methods which will enable a hydrogen storage system that meets DOE 2010 goals**

- **Project completion in three years**

- **Deliverables:**
  - **One kilogram of optimized material**
  - **Potential manufacturing process**
  - **Design for a hydrogen storage system**
  - **Documentation**

- ***Note: Projected Start Date = May 1, 2004***

Budget

	Total Budget	FY-2004	FY-2005
Total	$ 4,985,618	$ 1,569,954	$ 1,918,024
DOE	$ 2,000,000	$ 550,000	$ 814,229
Contractor	$ 2,985,618	$ 1,019,954	$ 1,103,795
UOP	$ 2,910,618	$ 1,009,537	$ 1,078,795
Ford (In-Kind)	$ 75,000	$ 10,417	$ 25,000

Technical Barriers and Targets

- **DOE Technical Barriers for On-Board H_2 Storage:**
  - **A. Cost**
  - **B. Weight and Volume**
  - **D. Durability**
  - **E. Refueling Time**
  - **M. Hydrogen Capacity and Reversibility**
  - **N. Lack of Understanding of Hydrogen Physisorption and Chemisorption**

- **DOE H_2 Storage System Technical Targets for 2010:**
  - **Useable Specific Energy from H_2: 2.0 kWh/kg**
  - **Useable Energy Density from H_2: 1.5 kWh/L**
  - **H_2 Delivery Temperature Range: -30 to 100°C**
  - **Cost: $4/kWh**
  - **Cycle Life: 1000 Cycles**
  - **Refueling Time: < 5 Minutes**

Technical Approach

- **Identify H_2 Storage Material Enabling DOE Targets**
  - **Virtual HT Screening of New Materials & Catalysts**
    - **Molecular modeling using classical & first-principles models**
    - **Identify candidates → guide experimental program**
  - **Combinatorial Synthesis & Screening**
    - **Medium-Throughput (8x, 2004) → High-Throughput(48x, 2005+)**
  - **Extend Combi-Informatics**
    - **Add new unit operations, data management & analysis**
  - **Extensive Testing, Characterization and Modeling of Leads**
    - **Scale up best leads to 50g, characterize & test at Univ. Hawaii**
    - **Increased Understanding of Promoted Complex Hydrides**
- **Demonstrate Viability for Commercial Application**
  - **Scale-Up Material Meeting Targets to 1 kg**
  - **Identify Potential Commercial Manufacturing Route**
    - **Leverage UOP's expertise in materials commercialization**
  - **Design H_2 Storage System**
  - **Perform Cost Estimates**

Project Safety

- **Safety issues identified during FMEA:**
  - **Complex Hydrides may be Water-Reactive and Pyrophoric**
  - **High Pressure Operation during Re-Hydriding [60-120 bar]**
- **Approach:**
  - **FMEA for equipment and procedures reviewed with UOP HS&E department**
- **Key Safety Procedures Identified:**
  - **(1) Extensive documentation of synthesis procedures**
  - **(2) Manipulate materials inside glove box where possible**
  - **(3) Solvent purification using solid treaters instead of distillation**
    - **Avoids potential ignition source**
  - **(4) Disposal of unused or spent hydrides:**
    - **Removable material: pack under N_2 + Mineral Oil → Disposal**
    - **Material adhering to reactors, etc: Deactivate under N_2 with T-Butanol > Ethanol > Water → Disposal**
  - **(5) Manufacturer's safety systems augmented with added reliefs**

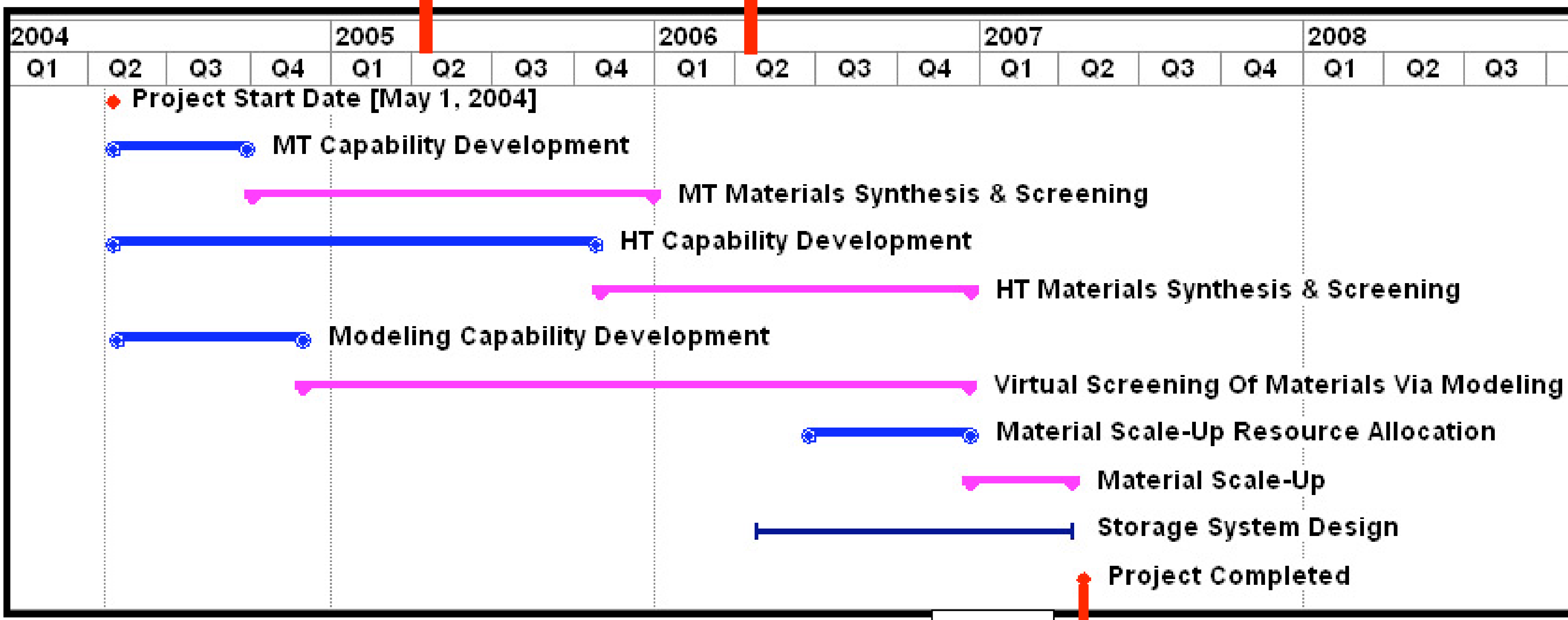
Project Timeline, Major Milestones

Hydride/Catalyst > state-of-the-art [Reversible Capacity, Temperature], Downselect Na, Li, Mg-Alanates

Hydride/Catalyst approaching DOE system targets, Downselect Be, Ca, B, Ga, and In hydrides

Yr-1

Yr-2



Yr-3

1 kg Hydride/Catalyst @ DOE system targets

Technical Accomplishments/Progress

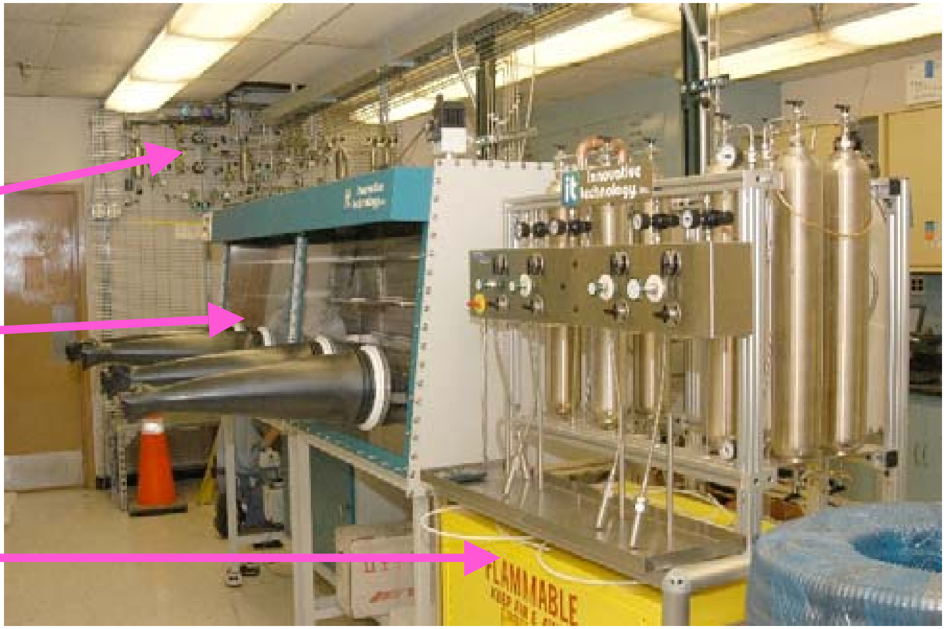
- **Projected Start Date = May 1, 2004**
- **Pre-Program Accomplishments:**
  - **Created laboratory for inert-gas materials synthesis**
  - **Purchased & installed equipment for medium-throughput synthesis and testing**
  - **Began model Development**

Not shown: Planetary Mills, 8-Reactor Assay

Gas Manifold

Synthesis Glove Box

Solvent Purification System



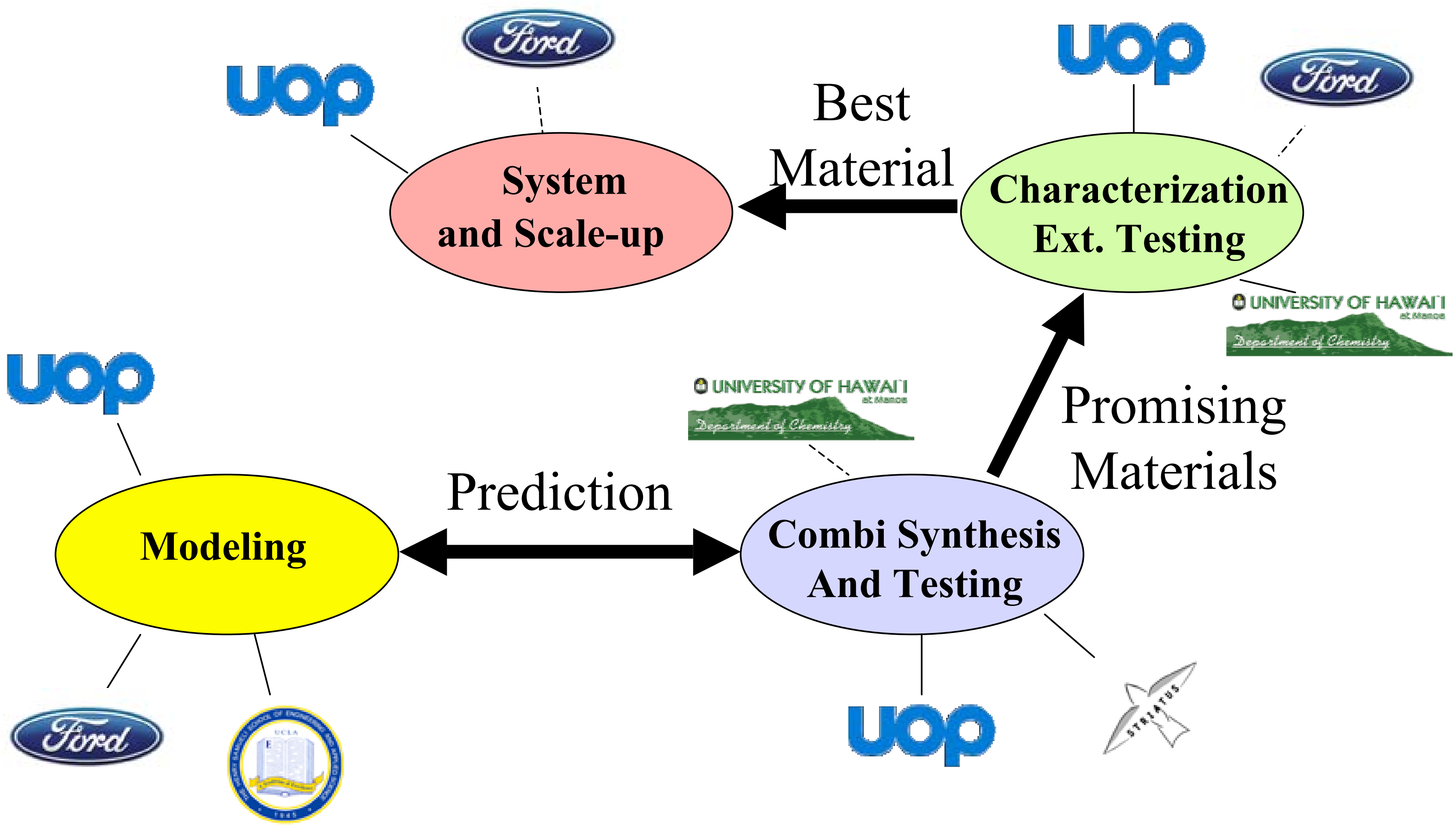
Interactions & Collaborations

DOE Project Manager

UOP
Dave Lesch – Project Manager
Adriaan Sachtler – Team Leader, Testing
John Low – Modeling
Greg Lewis – Synthesis
Doug Galloway – Characterization
Leon Halloran – Characterization
Yune Le – Combi Synthesis
Paul Dosek – Combi Testing

Ford	**UCLA**	**U of Hawaii**	**Striatus**
Chris Wolverton	**Vidvuds Ozolins**	**Craig Jensen**	**Laurel Harmon**
Modeling	**Modeling**	**Char/Testing**	**Informatics**

Role of Participants



Future Work - Year One Milestones

	Milestone	Outcome
Q1	Refine technical requirements	Target specifications for hydride/catalyst combinations defined
Q2	Develop and validate medium throughput (parallel) synthesis and testing tools	Metal hydride synthesis and screening (8 in parallel), validated against literature, Univ. Hawaii data
Q3	Develop and validate high throughput (parallel) characterization tools	Characterization methods (48 in parallel), validated against lab-scale measurements
Q3	Develop theoretical methods to predict stable hydride mixtures	Collection of stable hydride phases identified using molecular mechanics, validated by first-principles modeling, and available for experimental follow-up
Q4	Design and construct the high throughput synthesis and testing tools	High throughput systems constructed
Q4	Phase I hydride/catalyst screening completed	At least one hydride/catalyst combination that exceeds state-of-the-art identified

Year Two Milestones

	Milestone	Outcome
Q2	High throughput synthesis and testing implemented	HT synthesis and screening (48 in parallel) operational and validated using known materials
Q4	Modeling extended to catalysts	Model descriptors have been identified that correlate with reaction rates over catalyzed materials. Models have been validated using known catalyst systems and are ready to search for new systems.
Q4	Phase II hydride/catalyst screening completed	At least one hydride/catalyst combination that approaches DOE targets. This material has been validated at Univ. Hawaii
Q4	Improved mechanistic understanding	Fundamental studies at the Univ. Hawaii have increased the understanding of hydride and catalysts.

Year Three Milestones

	Milestone	Outcome
Q3	Candidate hydride identified and optimized	Candidate hydride/catalyst combination has been identified and optimized
Q4	Optimum hydride has been scaled up	A 1-kg quantity of the optimum hydride has been prepared and certified by testing
Q4	Prototype hydrogen storage system designed	Completed prototype design suitable for transportation application
Q4	Engineering and economic studies completed	Engineering and economic analyses to assess the commercial viability of a vehicle hydrogen storage system comprising the optimized material, a prototype storage system, and potential commercial manufacturing route

Go/No-Go Decision Points

- **Year One**
  - **Validation and Demonstration of VHTS (Molecular Modeling)**
  - **Validation and Demonstration of Medium Throughput Combinatorial Tools**
- **Year Two**
  - **Demonstration of High Throughput Combinatorial Tools**
  - **Identification of New Materials Approaching DOE Targets**

Summary

- **Virtual High Throughput Screening to select candidate complex hydrides with improved thermodynamics.**
- **Combinatorial methods to synthesize and screen candidates**
- **First Principles Calculations and Advanced Characterization to Understand Catalysts**
- **Scale-Up Material Enabling System Targets to 1 kg**
- **Identify Potential Commercial Manufacturing Route**
- **Design H_2 Storage System**
- **Perform Cost Estimates**
- **Improved material will enable a system meeting 2010 targets.**