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Fuel Cell and Hydrogen Research
Award No. DE-FG36-04GO14224

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Objectives

- **Task 1: Hydrogen Production**
  - Investigate a thermochemical cycle, biomass gasification, a photoelectrochemical device, an electrocatatlytic method, and a solid state electrolysis system.
- **Task 2: Hydrogen Storage**
  - Investigate transition metal hydrides, nano-structured materials (nano-composite conducting polymers), and hydrogen storage components designed for manufacturability
- **Task 3: Fuel Cells**
  - Investigate PEM and electrode improvements, water and thermal management, and construct a testing facility
- **Task 4: Hydrogen Demonstration Project**
  - Create demonstration using solar power to generate hydrogen for storage and conversion

First Year Budget
8/1/04 – 7/30/05

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University of South Florida - No. DE-FG36-04GO14224

YEAR 1			Funds Requested by Proposer	Funds Submitted as COST SHARE
A. SENIOR PERSONNEL: PI, Co-PIs	10		$135,247	$61,861
B. OTHER PERSONNEL				
1. POST DOCTORAL ASSOCIATE	3		$60,000	$3,000
2. OTHER PROFESSIONALS	1		$37,000	$0
3. GRADUATE STUDENTS	8		$125,000	$0
4. UNDERGRADUATE STUDENTS	3		$6,000	$6,000
5. ADMINISTRATIVE	0		$0	$0
TOTAL SALARIES AND WAGES (A+B)			$363,247	$70,861
C. FRINGE BENEFITS (Insurance)			$31,386	$10,507
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)			$396,108	$81,368
D. PERMANENT EQUIPMENT				
TOTAL EQUIPMENT			$178,500	$100,000
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)			$18,000	$0
2. INTERNATIONAL			$0	$0
F. OTHER DIRECT COSTS				
1. RESEARCH RELATED MATERIALS AND SUPPLIES			$120,000	$0
2. PUBLICATION, DOCUMENTATION, AND DISSEMINATION COSTS			$2,000	$0
3. SUBAWARD Yogi Goswami (University of Florida)			$784,951	$199,280
4. SUBAWARD Elena Shembel (Ener1, Inc)			$79,078	$19,795
5. SUBAWARD Clovis Linkous (University of Central Florida)			$78,525	$19,561
6. OTHER TUITION — FULL RATE P/HR: IN=$210 Out=$779; WAIVER RATE P/HR: IN=$171 OUT=$713 (171, 713)	#Students>>> IN 4	OUT 4	#Hours 18	
			$63,648	$0
TOTAL OTHER DIRECT COSTS			$1,128,202	$238,636
G. TOTAL DIRECT COSTS (A THROUGH G)			$1,720,810	$420,004
H. F&A (INDIRECT) COSTS - SPECIFY RATE	Base	Rate	F&A Costs	
yr1 Modified TDC	$536,108	45%	$241,248	
Cost Share Unrecovered overhea	$81,368	45%	$70,366	
TOTAL F&A COSTS			$241,248	$70,366
I. TOTAL DIRECT AND F&A COSTS (G+H)			$1,962,058	$490,369
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS)			$0	$0
J. AMOUNT OF THIS REQUEST (I) OR (K MINUS I)			$1,962,058	$490,369

Hydrogen Production: Technical Barriers and Targets

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Project	Technical Barriers to be Addressed	Targets
Thermochemical Cycle	Thermochemical technology, solar capital cost	Lower operating temperatures of cycle to improve economics
Biomass Gasification	Feedstock cost and availability, efficiency of gasification, CO emissions	Maximize hydrogen yield and efficiency of process while reducing emissions
Solar Photoelectrochemical	Cost, efficiency, catalyst	Improve hydrogen production cost to ~$70/m^2
Solar Photocatalytic	Cost, efficiency, catalyst	Improve efficiency of water splitting while addressing cost
Solid State Ionic Conductor	Cost, efficiency	Reduce weight and operating temperatures of electrolyte system

Hydrogen Production: Thermochemical Cycle

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- Approach
  - The University of Tokyo Cycle #3 (UT-3) is among the most promising thermochemical cycles proposed for hydrogen production. The UT-3 cycle has the advantage of lower operating temperatures (1000 K) compared to other thermochemical cycles. The cycle uses a CaO/CaBr2/Fe3O4/FeBr2 matrix for the thermochemical decomposition of water.
  - Areas of interest are solid reactant formulation, reactor kinetics, cycle thermodynamic and solid reactant surface studies
- Timeline (Funding period 8/1/04 – 7/30/05)

Activity	**Qtr. 1**	**Qtr. 2**	**Qtr. 3**	**Qtr. 4**
Setting up Reactor Facility	X	X		
Setting Pelletizing Facility	X	X		
Studying CaO Reactor Kinetics			X	
Studying CaBr Reactor Kinetics				X
Testing Pellet Performance			X	X

Hydrogen Production: Biomass Gassification

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- Approach
  - The constructed system consists of a steam generator, gasifier, a catalytic reactor, and gas chromatographic analysis facilities.
  - Based on initial runs modifications have been identified for *in situ* reduction of catalysts before each catalytic run, improvement to the gas analysis facility to increase sensitivity to hydrogen and analysis speed
  - Areas of interest are pretreatment of feedstock, catalyst improvement, and thermodynamic analysis
- Timeline (Funding period 8/1/04 – 7/30/05)

Activity	**Qtr. 1**	**Qtr. 2**	**Qtr. 3**	**Qtr. 4**
Gasifier &Analysis Facility Improvements	X	X		
Baseline testing		X	X	
Catalyst Reactor Assembly	X	X		
Catalyst Development			X	X
Thermodynamic Analysis	X	X	X	X

Hydrogen Production: Solar Photoelectrochemical

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- Approach
  - The use of solar cells to split water has been under study as a means of meeting the hydrogen supply
  - Start with Si since it is a proven technology and then investigate CIGS for lower cost which would then be targeted for a second generation
  - The proposed solar cell photocatalyst is CdSe. It has a band gap of 1.7 eV which is an ideal match to Si or CIGS. A critical part of the structure is the middle contact which will be tin oxide. This serves as the tunnel junction or recombination plane between the two devices, and must be transparent. The TO/Si device is a p/n heterojunction, and efficiencies of 14 – 15% have been reported in the literature for such structures
- Timeline (Funding period 8/1/04 – 7/30/05)

Activity	**Qtr. 1**	**Qtr. 2**	**Qtr. 3**	**Qtr. 4**
Representative TC/Si solar cell	X	X		
Representative CdSe/Si tandem solar cell		X	X	X

Hydrogen Production: Solar Photocatalytic

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- Approach
  - Photocatalytically split water using TiO_2 as the catalyst
  - TiO_2 will be the focus of studies, particularly the effort to enhance its photocatalytic activity by various methods, including size optimization, surface modification, and doping
- Timeline (Funding period 8/1/04 – 7/30/05)

Activity	**Qtr. 1**	**Qtr. 2**	**Qtr. 3**	**Qtr. 4**
Sol-gel and sputtering system facilities setup system/retrofit for dopant	X	X		
Contact structure development	X	X	X	X
Band structure alignment characterization w/ dopants via UPS			X	X
Mechanistic studies via TPD/TGA			X	X
Catalyst characterization			X	X
Testing and optimumization				X

Hydrogen Production: Solid State Ionic Conductor

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- Approach
  - Metallurgical and semiconductor processing techniques will be applied to known solid acid electrolyte materials to prepare strong and sturdy thin film electrolytes
  - New materials will be sought and investigated.
  - Catalysts and surface treatments will be applied to attempt to increase power densities.
- Timeline (Funding period 8/1/04 – 7/30/05)

Activity	**Qtr. 1**	**Qtr. 2**	**Qtr. 3**	**Qtr. 4**
Film Preparation	X	X	X	X
Cell Fabrication	X	X		
New Materials			X	X
Current Density Enhancement				X
Performance and Stability Study			X	X

Hydrogen Storage: Technical Barriers and Targets

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Project	Technical Barriers to be Addressed	Targets
Transition Metal Hydrides	Cost, weight and volume, efficiency, durability, hydrogen capacity and reversibility, Physisorption and Chemisorption	Address technical barriers to met DOE targets
Nano-Structured Materials (nano-composite conducting polymers)	Cost, weight and volume, efficiency, durability, hydrogen capacity and reversibility, Physisorption and Chemisorption	Address technical barriers to met DOE targets
Hydrogen Storage Components Designed for Manufacturability	Weight and Volume, Durability	Develop nanofoil fabrication and coiled packaging

Hydrogen Storage: Transition Metal Hydrides

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- Approach
  - Develop transition metal complex hydrides suitable for high and low temperature applications.
  - Absorption and desorption kinetics will be evaluated by optimizing the experimental parameters
  - The thermodynamic and kinetic characteristics of Mg2FeH6 will be optimized by Na/Li substitution and Ti-catalyst doping on the metal lattice.
- Timeline (Funding period 8/1/04 – 7/30/05)

Activity	**Qtr. 1**	**Qtr. 2**	**Qtr. 3**	**Qtr. 4**
Chemical / mechano-chemical synthesis of Mg_2FeH_6 and characterization	**X**			
Titanium catalyst doping and substitution of alkali metal (Na/Li) on the host metal structure Mg_2FeH_6	**X**	**X**		
Hydrogenation/dehydrogenation kinetics and hydrogen storage capacity as obtained from PCT isotherm experiments		**X**	**X**	
Cyclic retention for the unmodified and modified Mg_2FeH_6		**X**	**X**	**X**

Hydrogen Storage: Nano-Structured Materials

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- Approach
  - Synthesis of conducting polymers
  - Structural modification of fullerene molecules by incorporating sodium or potassium ions
  - Functionalization of conducting polymer for coupling with modified fullerenes
- Timeline (Funding period 8/1/04 – 7/30/05)

Activity	**Qtr. 1**	**Qtr. 2**	**Qtr. 3**	**Qtr. 4**
Synthesis of various conducting polymers and its characterization	**X**			
Modification of fullerene structure and functionalization of conducting polymers	**X**	**X**		
Preparation and characterization of nano-composite conducting polymers encompassing modified fullerene and carbon nanotube.		**X**	**X**	
Hydrogenation and dehydrogenation results of nano-composite conducting polymers using Temperature programmed Desorption or Pressure-Composition isotherm apparatus.			**X**	**X**

Hydrogen Storage: Hydrogen Storage Components

- Approach
  - Develop nanofoil fabrication technique with nanometer-sized grain structure and large surface area relative to film thickness
  - This nanofoil will be coiled into a cylindrical form factor and sealed into a canister for cyclic hydrogen storage testing
- Timeline (Funding period 8/1/04 – 7/30/05)

Activity	Qtr. 1	Qtr. 2	Qtr. 3	Qtr. 4
Design a research and development plasma sputtering system with in situ foil handling components	X	X	X	
Qualify operation and functionality of sputter deposition on stationary substrates using standard metals: Al and Ti			X	
Demonstrate operation of foil/substrate handling system and placement into canisters				X

Fuel Cells: Technical Barriers and Targets

Project	Technical Barriers to be Addressed	Targets
PEM and Electrode Material Improvement	Durability, Heat Utilization, Electrode Performance, Cost	Decrease cost of PEMs while allowing better performance
Water and Thermal Management	Durability, Heat Utilization, Cost, Stack material and Manufacturing Cost	Demonstrate improved water and thermal management system
Testing Facility	Maintenance and Training Facilities, Stack material and Manufacturing Cost, Heat Utilization	Allow testing and characterization of fuel cells and related components

Fuel Cells:
PEM and Electrode Material Improvement

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- Approach
  - Prepare and evaluate hydrophilic nanopartical composites for PEMs
  - Prepare and evaluate ionomers based on engineering polymers for PEMs
  - Demonstrate high density sulfonation for PEMs
  - Dope electrodes with new catalysts and manufacture membrane electrode assembly
  - Demonstrate improved characteristics
- Timeline (Funding period 8/1/04 – 7/30/05)

Activity	**Qtr. 1**	**Qtr. 2**	**Qtr. 3**	**Qtr. 4**
Prepare and evaluate hydrophilic nanopartical composites	X	X	X	X
Prepare and evaluate ionomers based on engineering polymers	X	X	X	X
Demonstrate high density sulfonation	X	X	X	X
Dope electrodes with new catalysts and manufacture membrane electrode assembly	X	X	X	X

Fuel Cells: Water and Thermal Management

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- Approach
  - Assembly of stacks with improved design
  - Parametric testing of air flow rate, air humidity level, fuel humidity level, pressure, and temperature
  - Surface analysis of membranes after testing
  - Modeling of thermal losses
  - Design and manufacture effective heat removal
- Timeline (Funding period 8/1/04 – 7/30/05)

Activity	**Qtr. 1**	**Qtr. 2**	**Qtr. 3**	**Qtr. 4**
Modeling of thermal losses	X	X		
Parametric testing of air flow rate, air humidity level, fuel humidity level, pressure, and temperature	X	X	X	X
Design and manufacture effective heat removal			X	X
Assembly of stacks with improved design				X

Fuel Cells: Testing Facility

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- Approach
  - Identification of operating parameters for fuel cell units
  - Baseline testing with standard PEM fuel cells and high purity hydrogen
- Timeline (Funding period 8/1/04 – 7/30/05)

Activity	**Qtr. 1**	**Qtr. 2**	**Qtr. 3**	**Qtr. 4**
Identification of operating parameters	X			
Design of complete testing facility	X	X		
Procurement of components		X	X	X
Construction of complete testing facility			X	X

Hydrogen Demonstration: Study of Hydrogen Infrastructure

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- Develop comprehensive demonstration, R&D project that supports the development of:
  - Hydrogen infrastructure
  - Hydrogen production
  - Hydrogen storage
  - Hydrogen conversion (fuel cells)
- Project description: USF will utilize an existing 20 KW solar power station to provide power to electrolyze water. The subsequent hydrogen will be stored for fuelling purposes in vehicles or converted to power and supplied to the grid

- Technical Barriers to be addressed
  - Thermal management
  - Fuel cell power system benchmarking
  - Durability and cost
  - Maintenance and training facilities
  - Codes and standards
  - Hydrogen from renewable resources

Project Safety

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- The safety aspect for the hydrogen projects will be given a careful consideration by the project team under the supervision of the Division of Environmental Health and Safety of the Florida University system. Daily operation will adhere to the Chemical Hygiene Plan SOP (standard operating procedure) provided by EH&S.

Interactions and Collaborations

- University of Florida (Yogi Goswami; Ph.D.)
  - Thermochemical cycle, biomass gasification, transition metal complexes, water and thermal management, testing facility
- University of South Florida's Center for Ocean Technology
  - Hydrogen storage components designed for manufacturability
- University of Central Florida (Clovis Linkous; Ph.D.)
  - Solid polymer electrolytes
- Ener1, Inc. (Elena Shembel; Ph.D.)
  - Ionomers based on engineering polymers

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