Discovery of Photocatalysts for Hydrogen Production

2003 DOE Hydrogen Review

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Berkeley, CA

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Off We Go…

"We are at the peak of the oil age but the beginning of the hydrogen age. Anything else is an interim solution. The transition will be very messy, and will take many technological paths .....but the future will be hydrogen fuel cells."

Herman Kuipers, Manager of Exploratory Research
Royal Dutch Shell

"General Motors absolutely sees the long-term future of the world being based on a hydrogen economy."

Larry Burns, Director of R&D, General Motors

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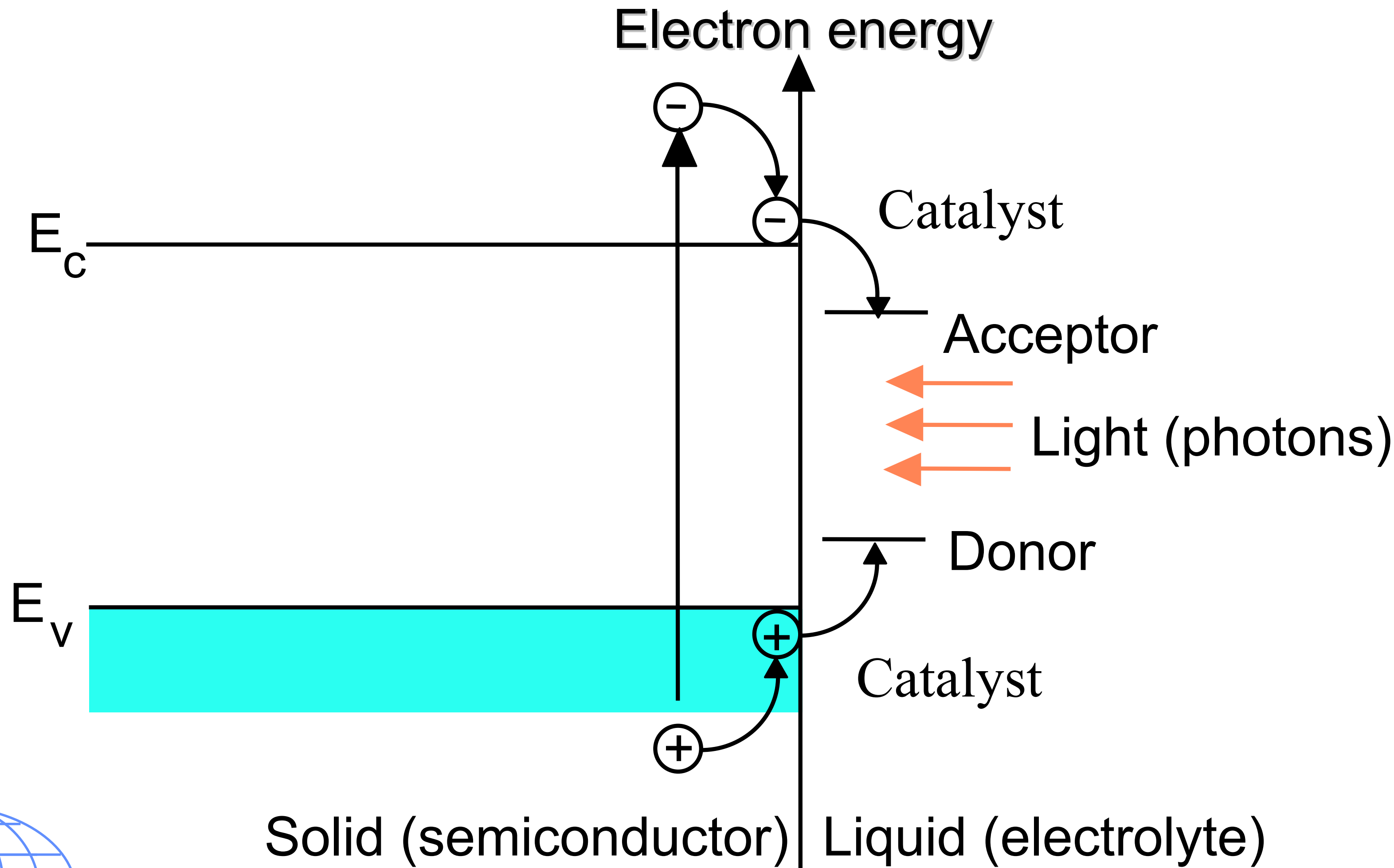
PEC 101



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Relevance/Objective: Technical Barriers

Key Technical Barriers are Materials and Systems Engineering Related

- **Efficiency (band gap and edges), Durability and Cost**

Materials need to be found that address these issues.

This project will assist in the identification of materials that directly address these barriers.

Specifically, the discovery of low cost materials with improved efficiency will be a driver to lower cost PEC hydrogen.

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Relevance/Objective: Technical Targets

Characteristics	2003 Status	2005 Target	2010 Target	2015 Target
Solar-to-hydrogen Efficiency	7%	7.5%	9%	14%
Durability	100 h	1,000 h	10,000	20,000
Cost	N/a	360	22	5

Targets for 2005 and 2010 involve sequential order of magnitude improvements in durability and modest improvements in efficiency.

Meeting these targets will require improvement of efficiency of existing highly durable oxide components, systems engineering to reduce cost of efficient multi-junction designs or a combination thereof.

The materials discovery required to meet the Technical Targets will be expedited by the use of high throughput screening tools being developed in this project. Furthermore, the inclusion of a partner with the means to produce commercially relevant amounts of materials will hasten the development required to make PEC hydrogen viable.

Approach

The goals of this project are to:

- Develop tools that will allow for the high throughput analysis of materials prepared with commercially relevant synthetic means with respect to PEC hydrogen.
- Use Neophotonics/NanoGram's laser pyrolysis to prepare new materials (composition/phase/particle size) for screening with respect to PEC hydrogen.

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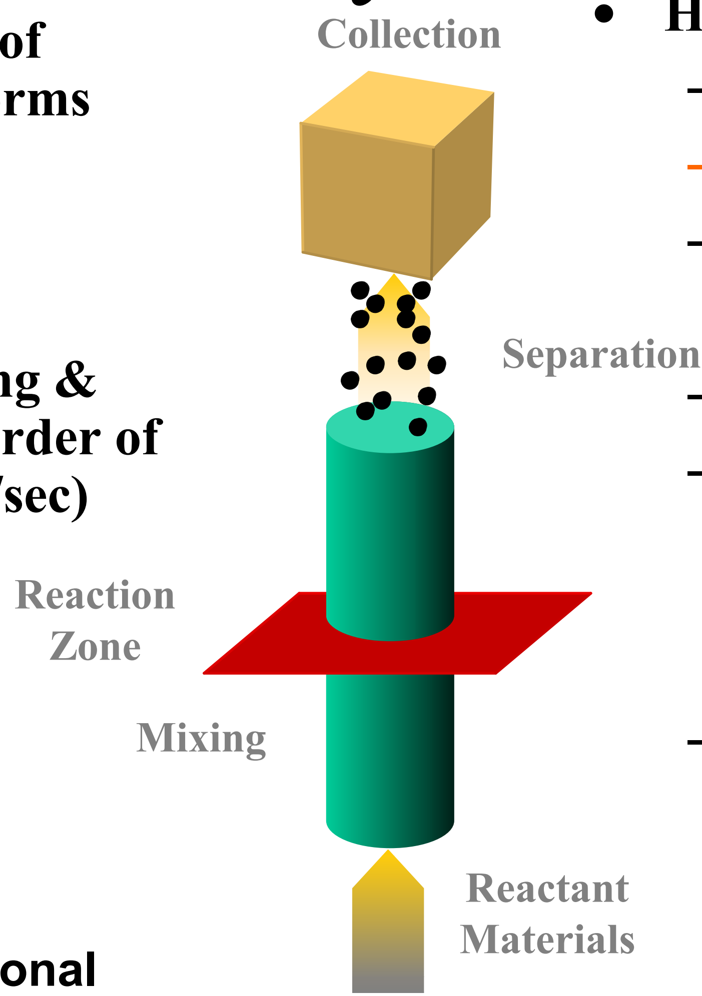
Laser-driven Nanoparticles Synthesis

- **Wide range of precursor forms**
  - **Gas**
  - **Vapor**
  - **Aerosol**
- **Rapid heating & quench (at order of 10^5 degrees/sec)**



- **Huge materials portfolio**
  - **Crystalline inorganics**
  - **Multi-element compounds**
  - **Tightly controlled size**
  - **High chemical purity**
  - **Oxide, sulfide, nitride, metal, phosphate, carbide, silicate inorganic compounds...**
  - **Rare earth-doping at high concentration**
    - **Scalable over 1kg/hr per equipment**

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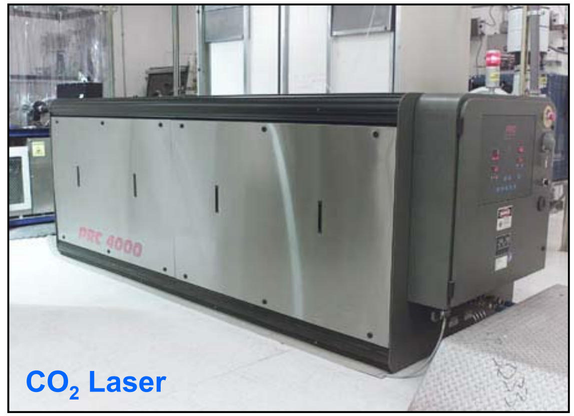
Scalability

High Volume Production System

LRD Reactor



CO_2 Laser

Controller

Scrubber System

Chemical Delivery System

- **Industrial; mass production**
  - **up to 10,000 wafers/year/system**
- **Fifth-generation technology**

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Project Timeline

Project initiated in October 2001 as three year effort to develop tools and investigate new materials.

Business decisions of partner on project resulted in year 1 being 17 months. Spending to date and funding requested are summarized below:

Source Year	1	2	3
DOE	250K	320K (0)	360K
Neophotonics/NanoGram	62K	80K	90K
Total	312K	400K	450K

Year 2 amount in parenthesis is funding received to date.

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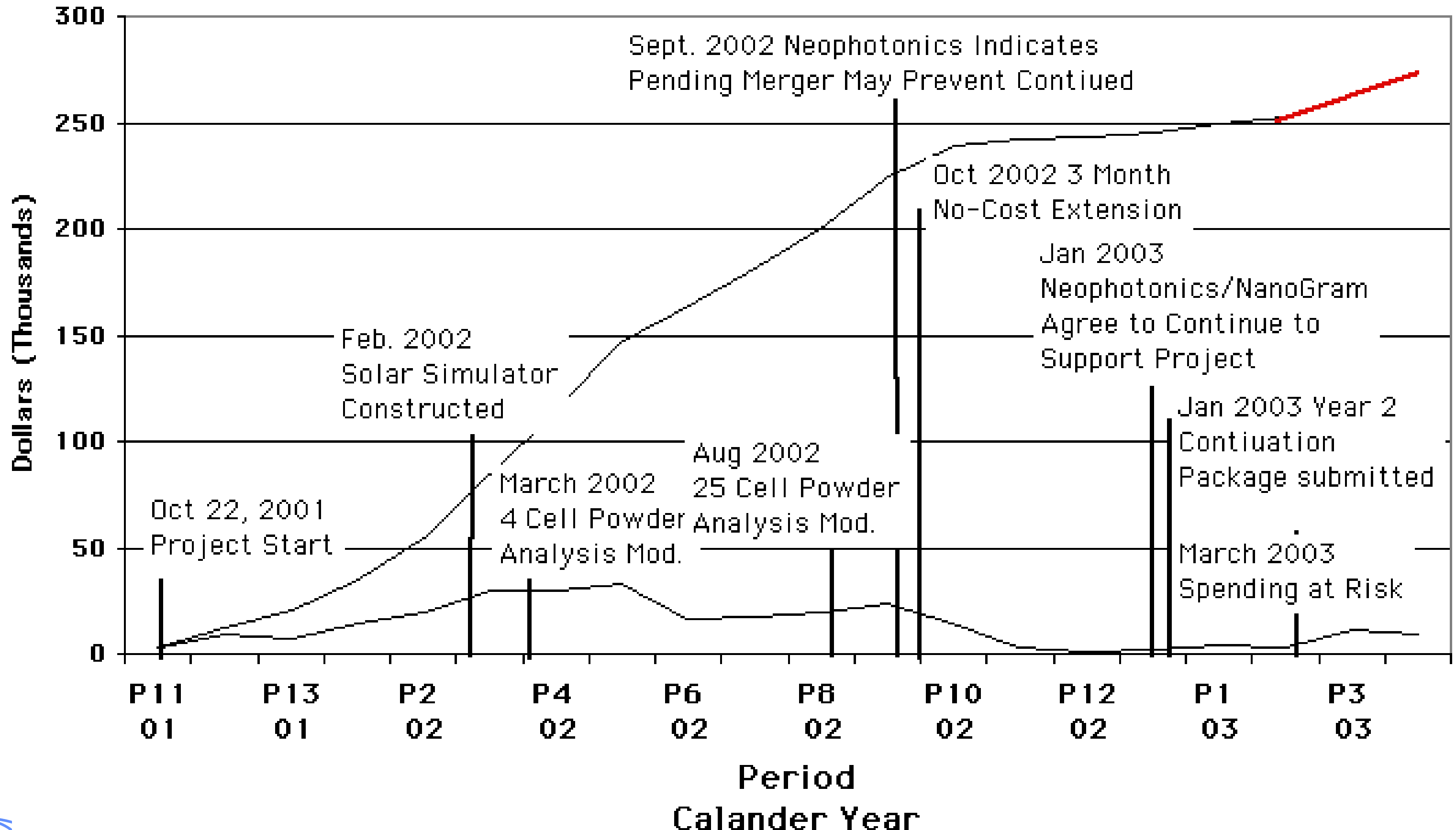
Timeline (cont..)



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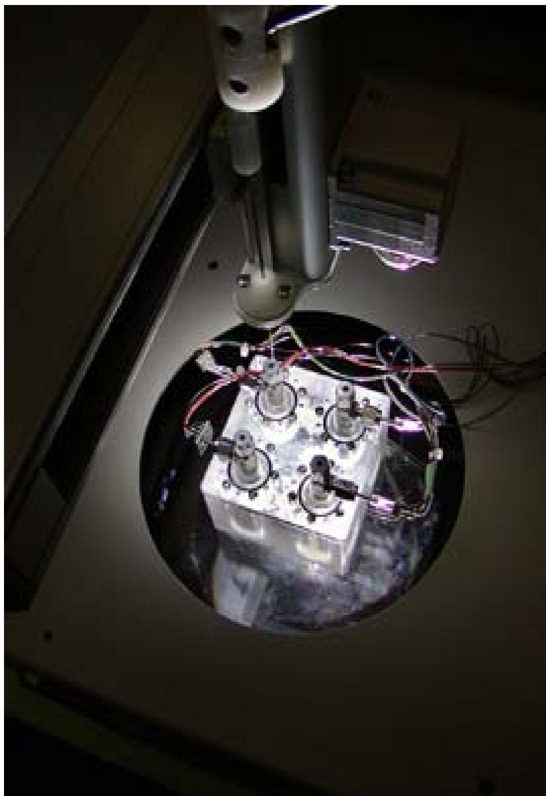
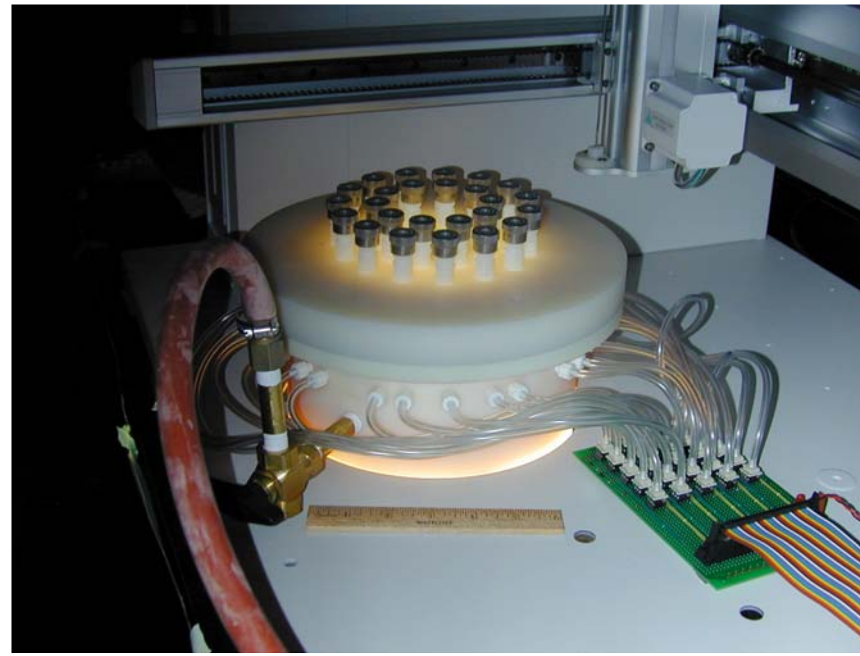
Accomplishments/Progress





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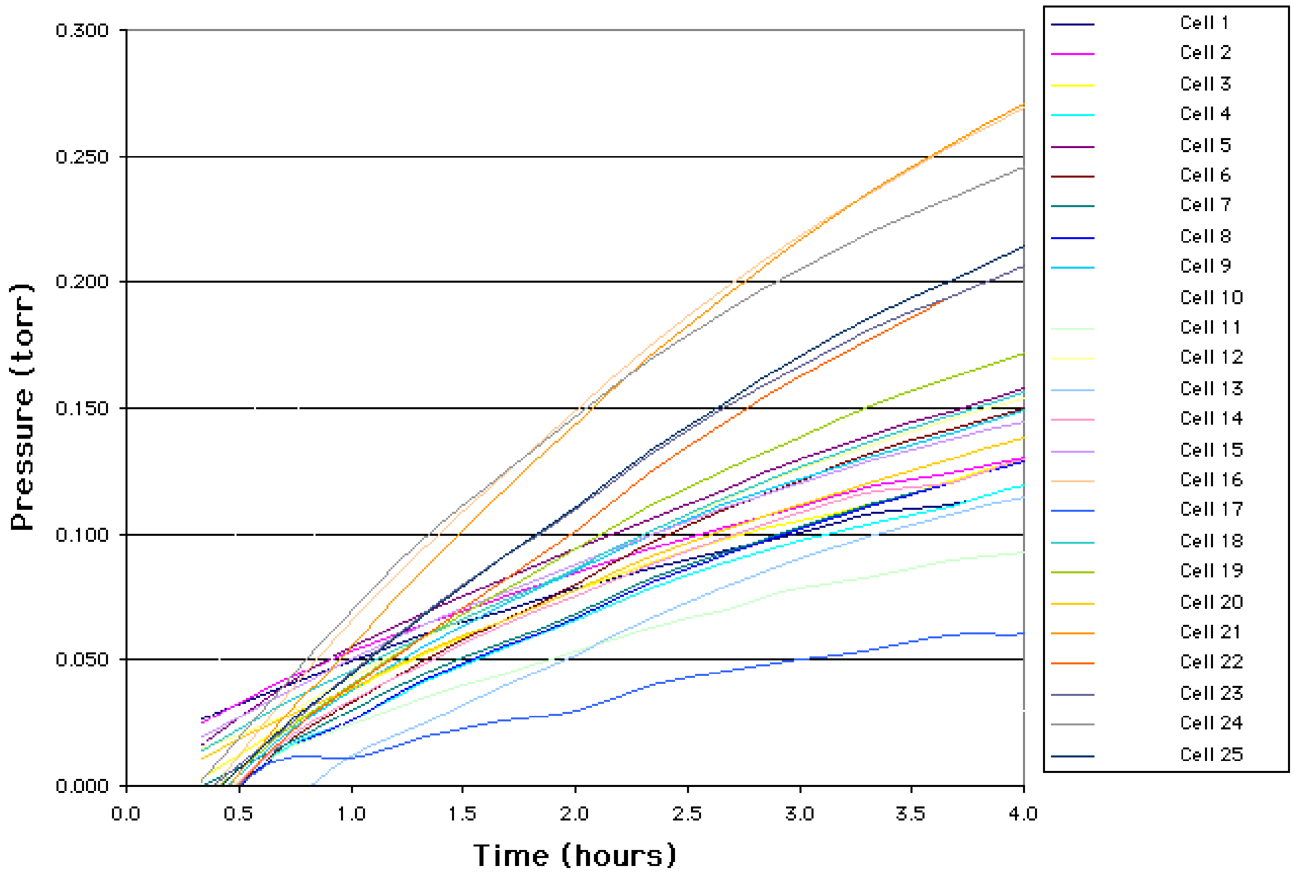
Accomplishments/Progress (cont.)



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Accomplishments/Progress (cont.)

Sample	median diameter, µm	Surface area, m2/gm
TDX-25	0.11	20.9
TDX-33	0.10	20.1
TDX-30	0.08	22.8
TDX-101	0.08	27.9
TDX-37	0.07	26.2
TDX-51	0.07	25.3
DIM76	0.07	38.0
TDX-50A	0.06	29.4
TDX-55	0.06	29.0
TDX-110	0.06	33.6
TDX-24	0.05	32.8
DIM57	0.04	52.5
DIM113	<0.03	56.0
DIM82	< 0.03	55.6

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Interactions/Collaborations

- Presentation at inaugural GCEP workshop
- Prof. Joop Schoonman, Delft University to visit SRI in early July to discuss potential collaboration
- Working on agreement with other DOE funded groups to share information and materials
- Materials transfer agreement available

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Detailed Plans for Year 2

- Task 1 Tools Development
  - **Debug powder module software for auto sampling**
    - **Early June 2003**
  - **Electrochemistry Analysis Module**
    - **Design review: May 2003**
    - **Fabrication: August 2003**

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Detailed Plans for Year 2 (cont.)

- Task 2. Analysis of Nanoparticulate-based PEC Systems
  - Analysis and characterization of Neophotonic (and SRI) generated materials
  - Based on results develop rationale design of future materials (elemental, phase, size)
  - Evaluate materials reported in literature
    - Synthesized at SRI
    - Submitted to SRI (Materials Transfer Agreement)

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Detailed Plans for Year 2 (cont.)

- Task 3. Generation of Database
  - Inclusion of validated data with sufficient information for reproduction in other labs
- Task 4. Modeling Feasibility
  - Survey existing programs for suitability in modeling material stability relevant to PEC production of hydrogen

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Detailed Plans for Year 2 (cont.)

Task Designation/Milestones	Year 2				Y3
	Q1	Q2	Q3	Q4	Q1
Task 1. Tools for the Development of Photoelectrochemical Systems for the Generation of Hydrogen.					
(a) Electrochemical analysis module, prototype design	▲				
(b) Prototype assembly		▲			
(c) Prototype Validation			★		
Task 2. Synthesis of Nanoparticulate-Based Photoelectrochemical Systems for Hydrogen Production Via Photolytic Water Splitting					
(a) Characterization of as received and modified materials (Y2 materials)				▲	
Task 3. Generation of Database of Experimental Results					
(a) Database setup	▲				
(b) Database implementation		★			
Task 4. Feasibility Study for the Generation of a Model to Predict Photoelectrochemical behavior of Nanoparticulate Semiconductor-Based Systems.					
(a) Survey existing modeling programs			▲		

▲ Subtask completion

★ Milestone completion

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Reviewers Comments

- Comments were overall very positive
- “Criteria for picking candidates needs to be done”

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Neophotonics Compositions Produced (Partial List)

Compositions Produced:

Amorphous Glass Materials

SiO_2, PSG, BPSG, GPSG

Elemental Metals

Fe, Ag, Ni, Co, Pt

Oxides

TiO_2, ZnO, VO_2, V_2O_3 , V_2O_5 , MnO, Mn_2O_3,
Mn_3O_4, MoO_3, NbO_2, Nb_2O_5, Y_2O_3, SnO, SnO_2,
SiO_2, Al_2O_3 , Fe_2O_3, Fe_3O_4

Complex oxides

$LiMn_2O_4$, $Li_2Mn_4O_9$, $Li_4Mn_5O_{12}$, $LiCoO_2$, $LiNiO_2$
$LiNi_{0.8}Co_{0.2}O_2$, $LiMn_{2-y}Al_yO_4$, $LiMn_{2-y}Co_yO_4$
$Li_4Ti_5O_{12}$, Y_2MoO_6, $Ag_2V_4O_{11}$, $BaMgAl_{10}O_{17}$:Eu

Carbon and Carbides

C, SiC, NbC, V_8C_7

Nitrides

Si_3N_4

Phosphates

$LiFePO_4$

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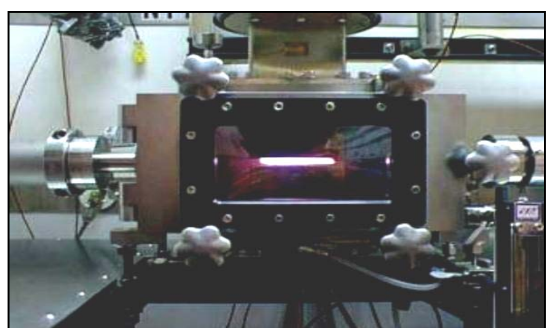
NPM™ NanoParticle Discovery System

C9000 Volume Production Module



Close-up: NanoParticle Laser Reaction Chamber

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Thank You, Stay Tuned

Slide by R. Smalley Presented at National Nanotechnology Initiative

- **ENERGY**
  is the single most important problem facing humanity today.
- **WE CAN SOLVE THIS PROBLEM**
  with revolutionary breakthroughs at the frontiers of Physical Sciences & Engineering, and particularly in Nanotechnology
- We need a new APOLLO PROJECT to do this.
- The problem is huge, but it is also a magnificent opportunity.
- Success will revolutionize the largest industry in the world, Energy.
- American boys and girls will enter the physical sciences to do this, inspired by their idealism, their sense of mission, and their desire to be "where the action is".
- In the process this new Apollo Project will produce a cornucopia of new technologies, and provide the underpinnings for vast new economic prosperity for the US and the world.

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